Tensor Networks & Entanglement

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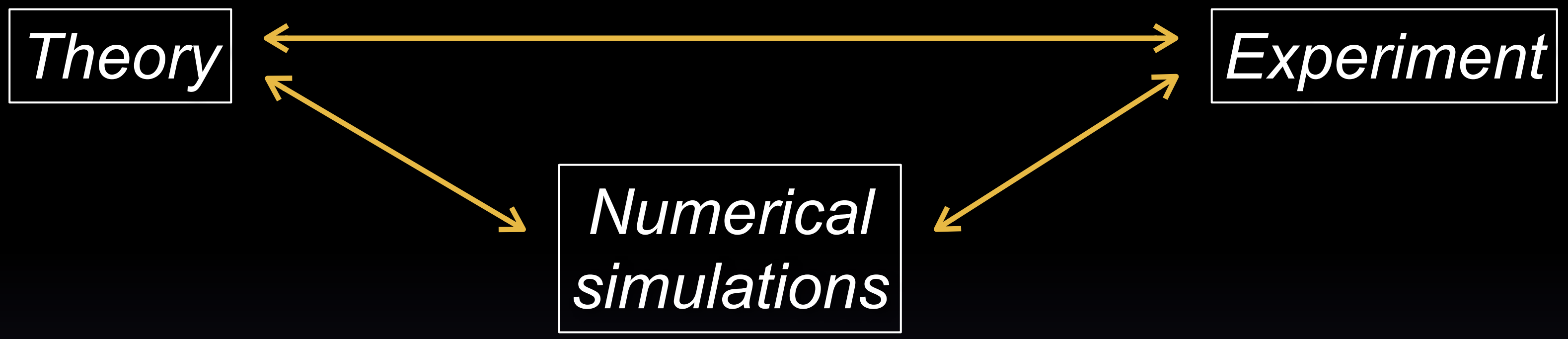
Motivation remarks



Numerical algorithms *(used as Tensor Networks)*

- *MPS* — *Matrix Product States*
- *PEPS* — *Projected-Entangled Pair States*
- *DMRG* — *Density Matrix Renormalization Group*
- *TEBD* — *Time Evolving Block Decimation*
- *HOTRG* — *Higher-Order Tensor Renormalization Group*
- *TPVF* — *Tensor Product Variational Formulation*
- *MERA* — *Multi-scale Entanglement Renormalization Ansatz*
- *CTMRG* — *Corner Transfer Matrix Renormalization Group*

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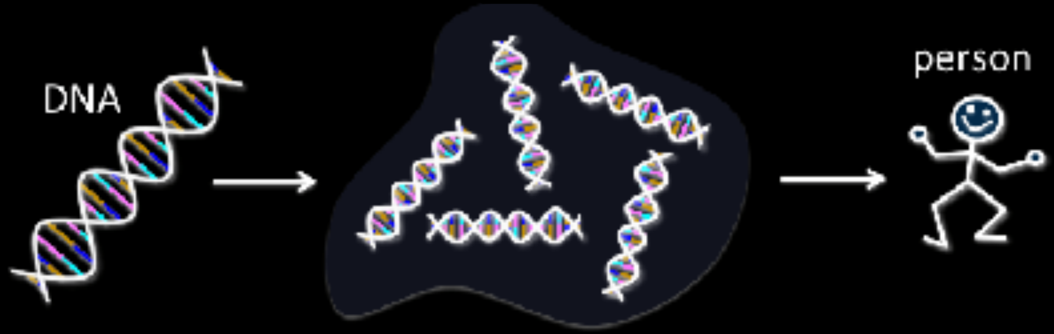
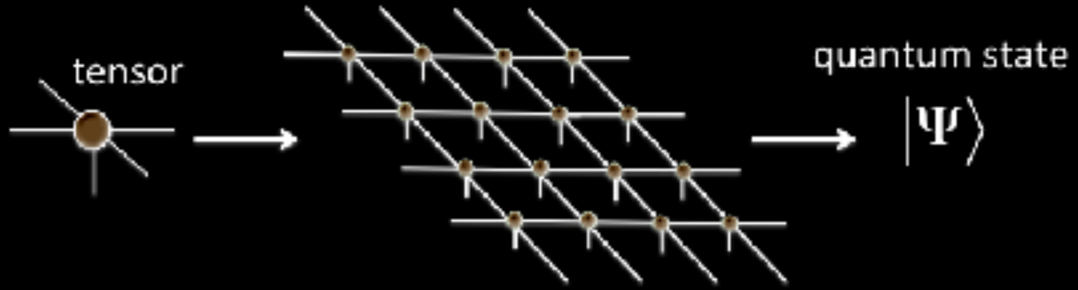
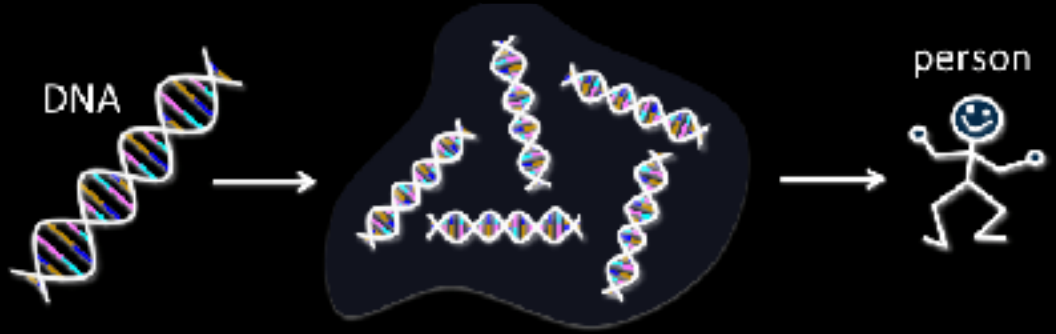
$$\approx |\psi\rangle$$


DNA
person


tensor
quantum state
$|\Psi\rangle$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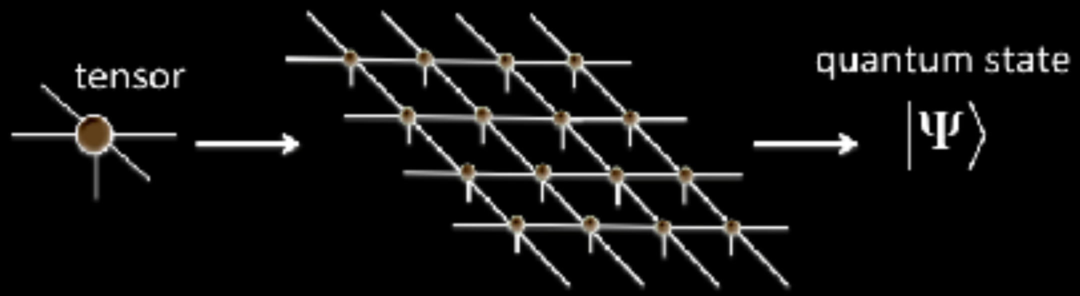
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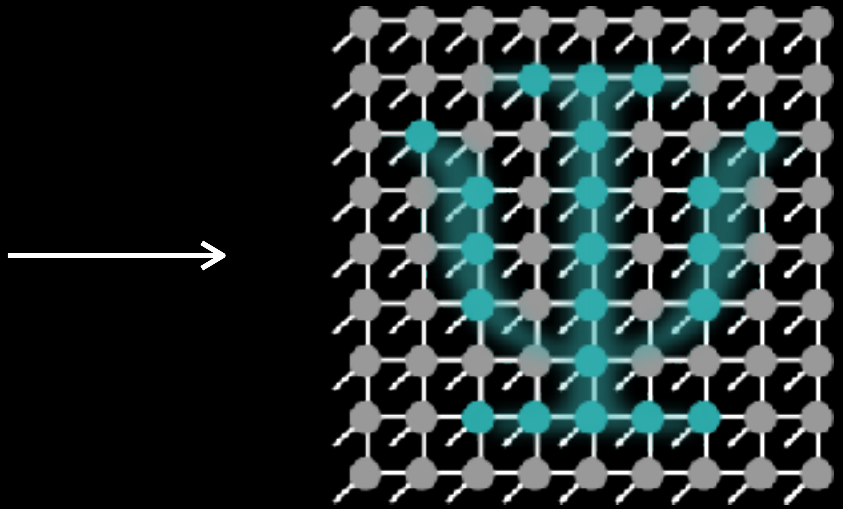

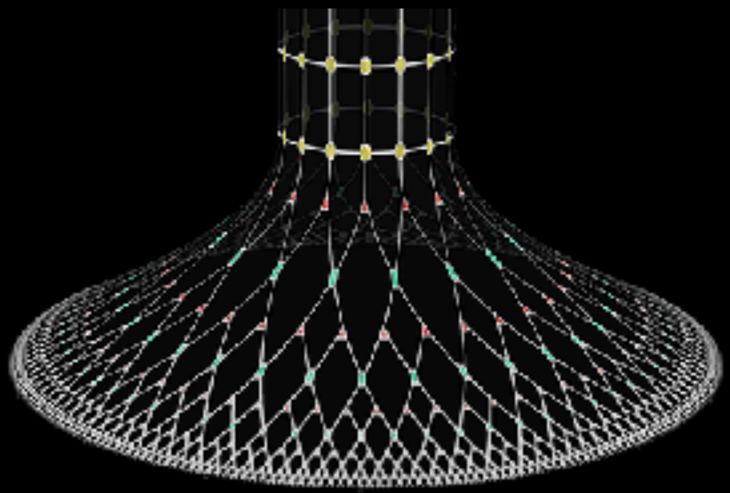

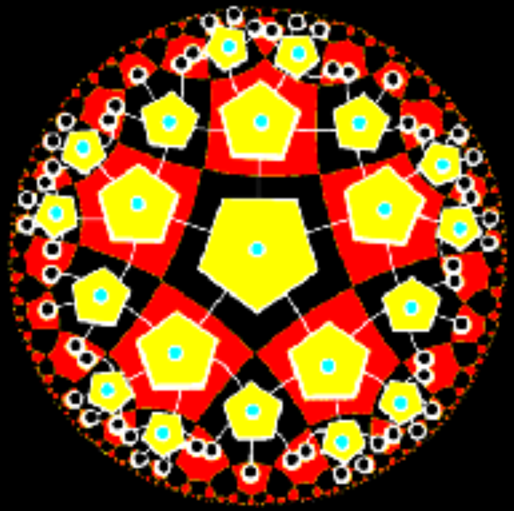

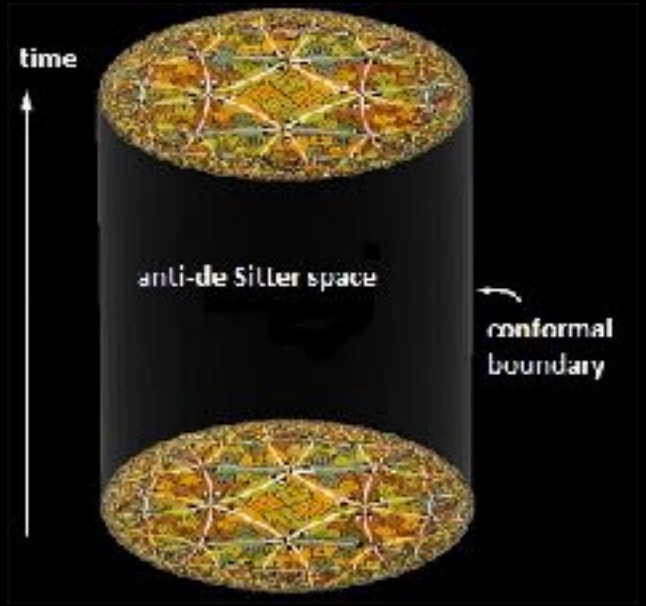
time
anti-de Sitter space
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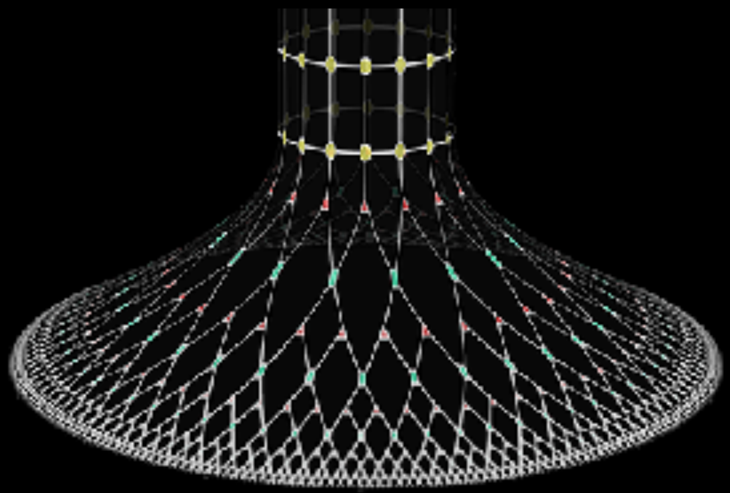

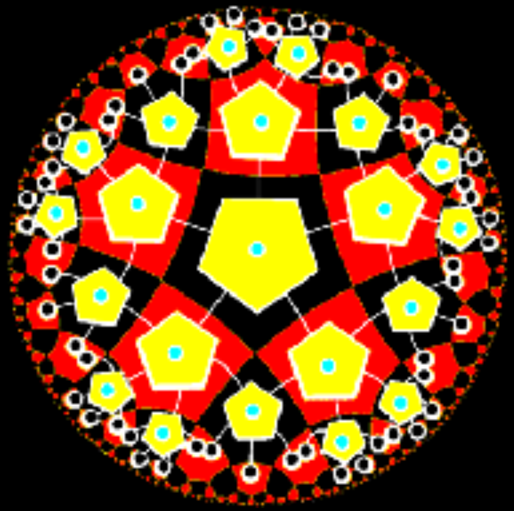

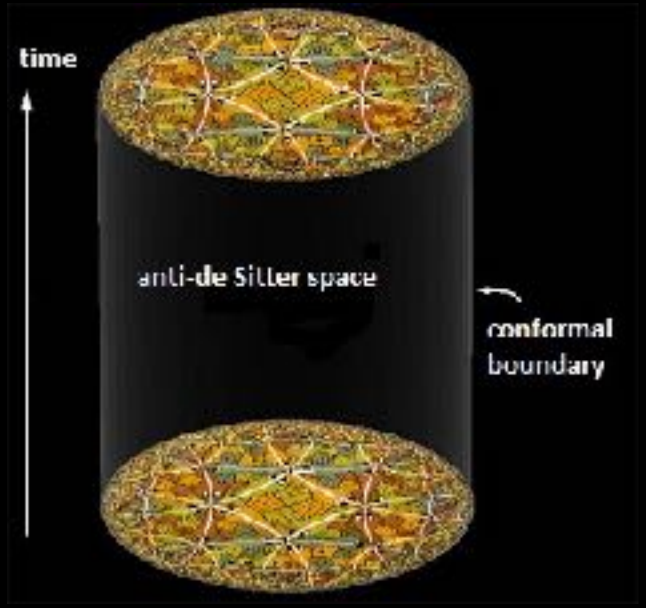
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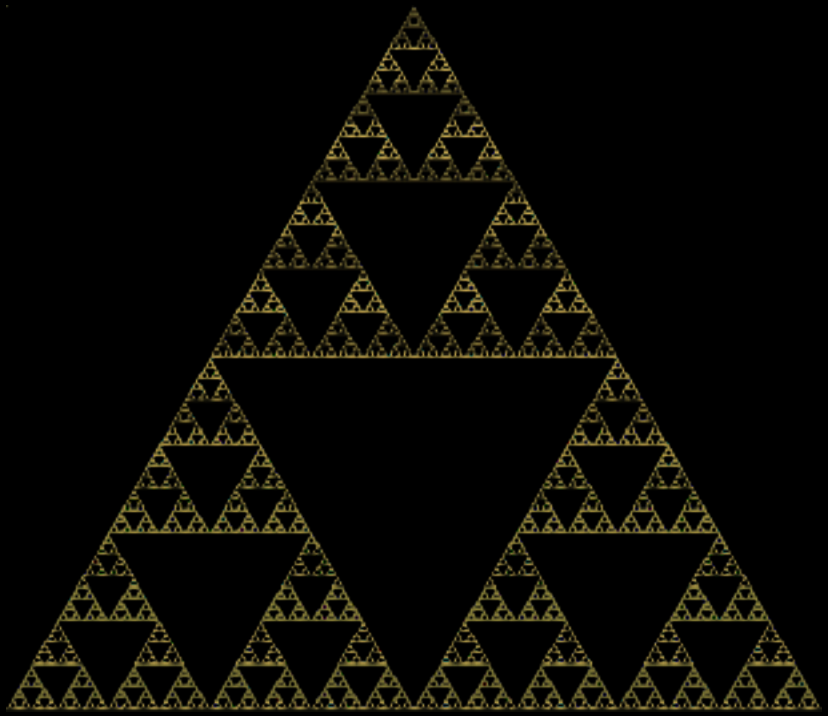

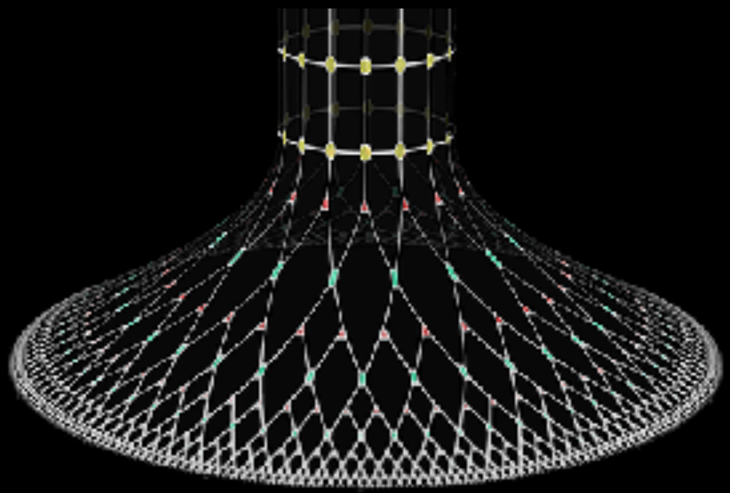

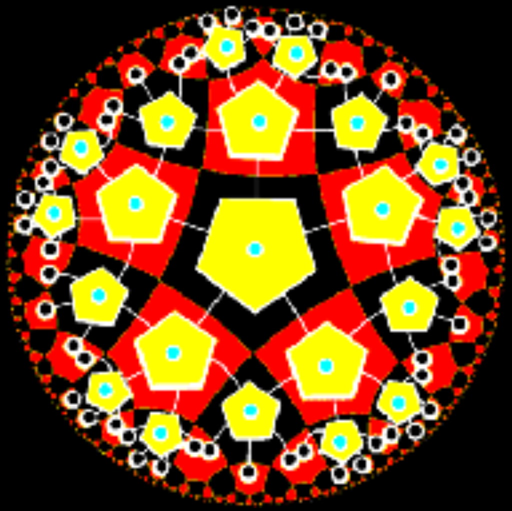

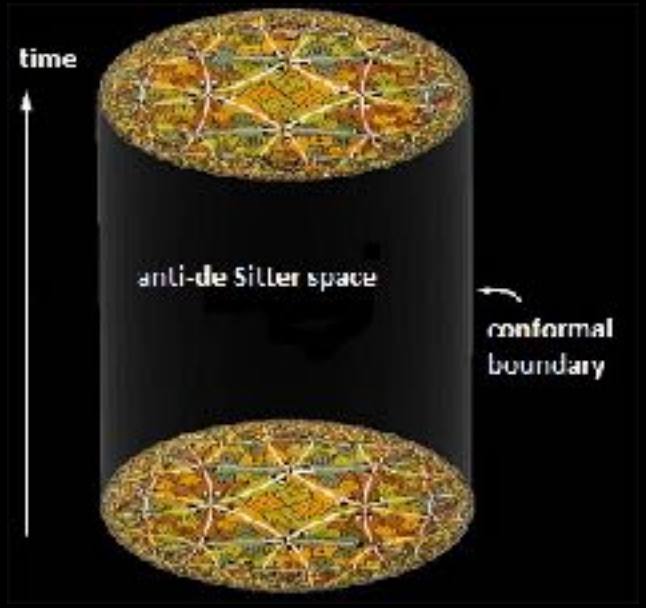

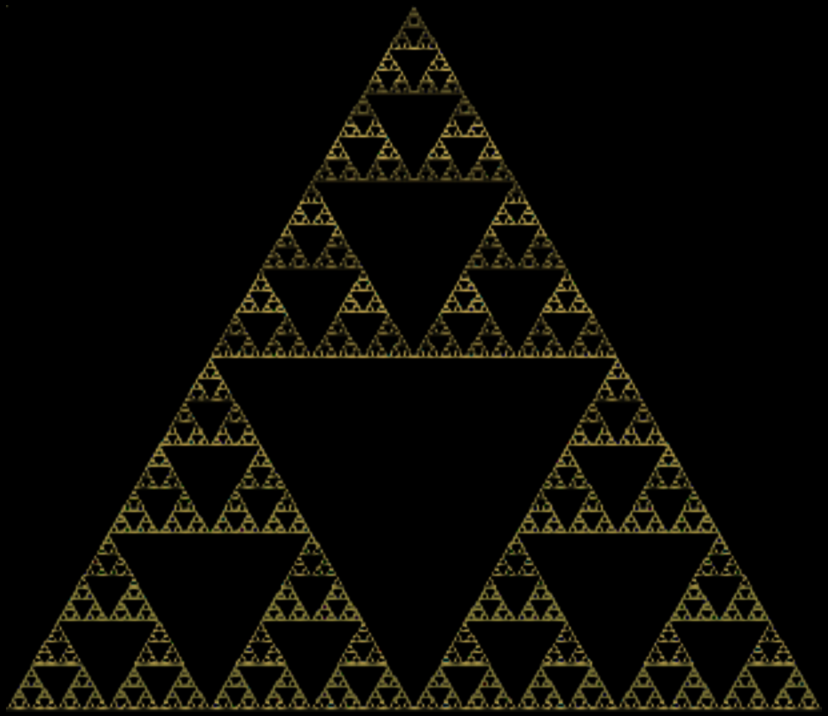

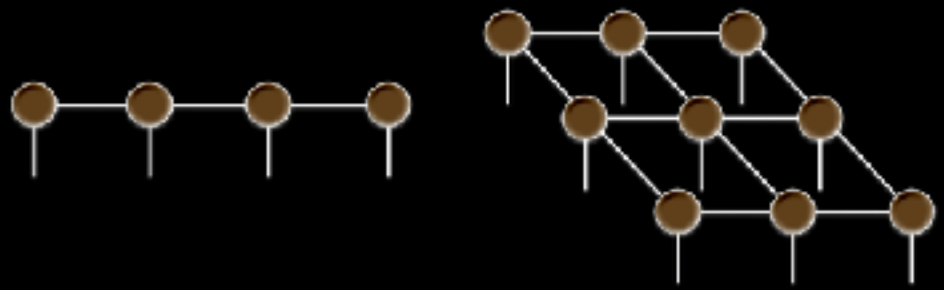

Matrix Product State → Tensor Product State

Quantum mechanics

Introduction to numerics

Introduction to solving quantum-mechanical problems

- ➢ Only a few simple systems are exactly (analytically) solvable!

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  - either analytically
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➢ Examples: Let us study the two simplest quantum systems

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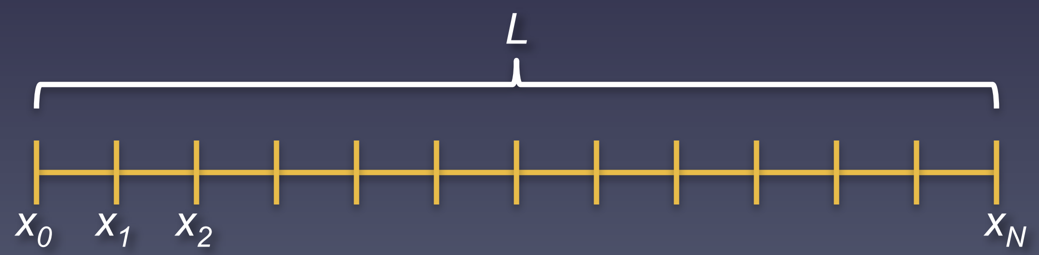
- Examples: Let us study the two simplest quantum systems

Discretization: $0 \le x \le L \to x_i = \frac{iL}{N}$ and $i = 0,1,2,\ldots,N$

$x \to x_i \to i$

$f(x) \to f(x_i) \to f_i$



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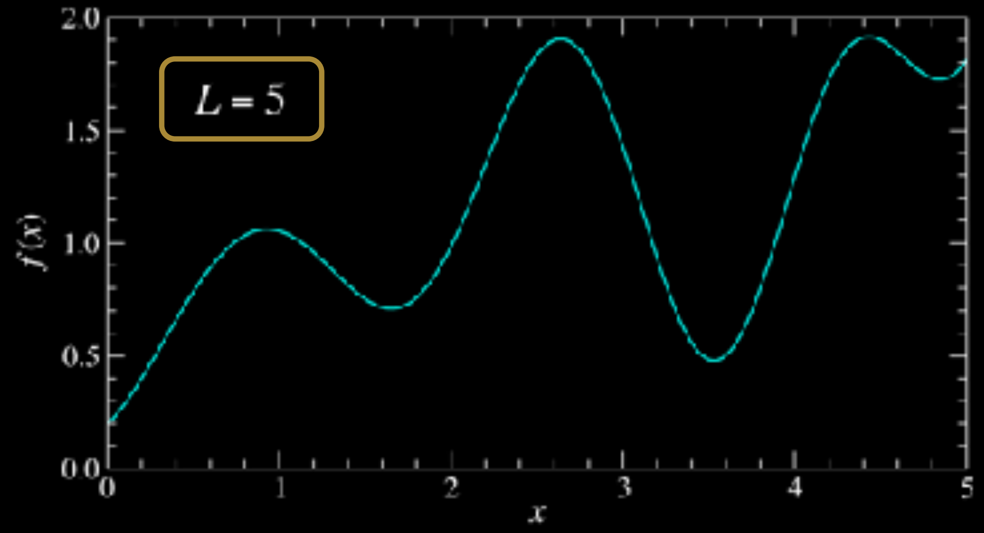

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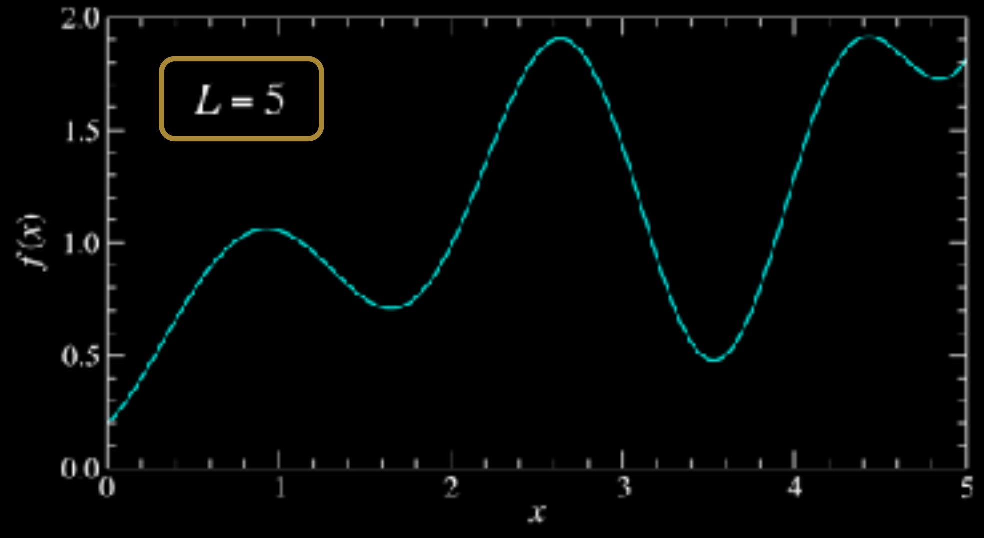

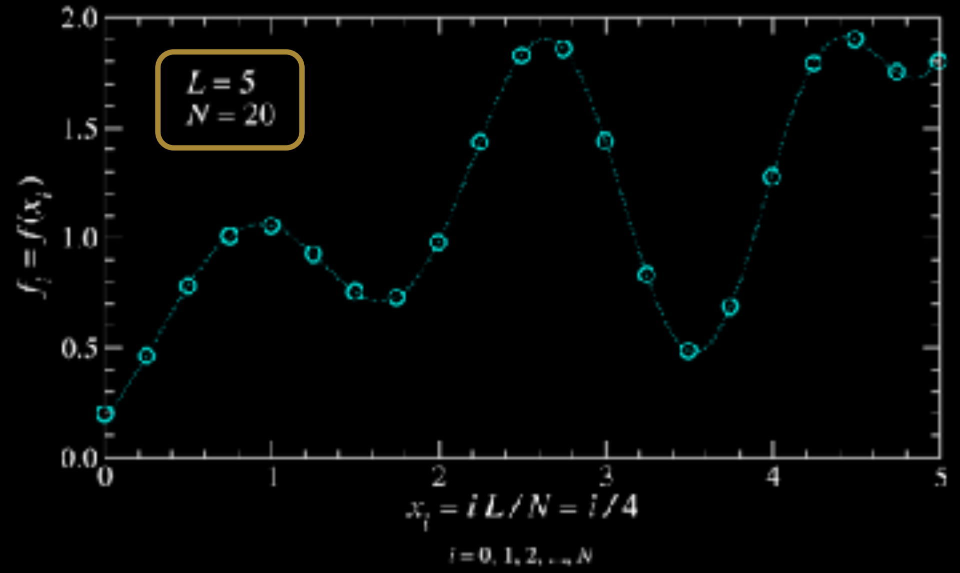

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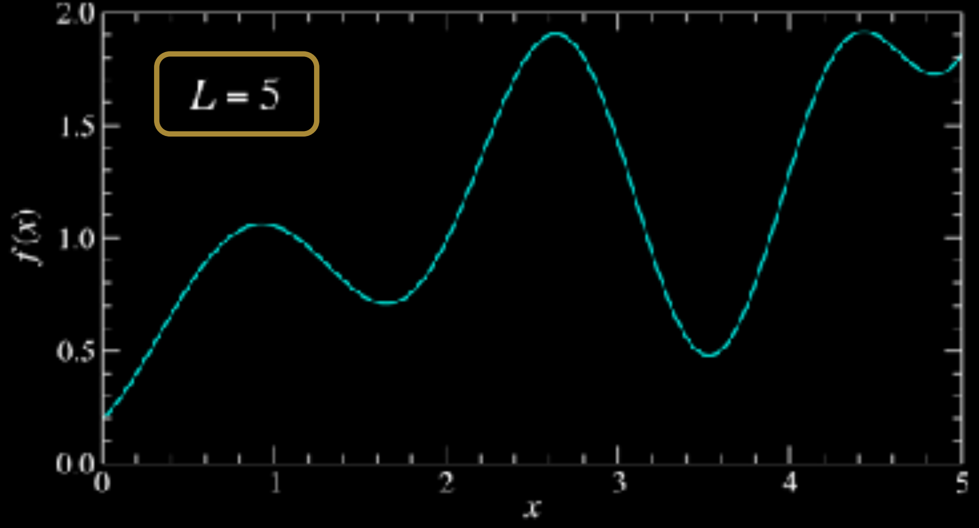

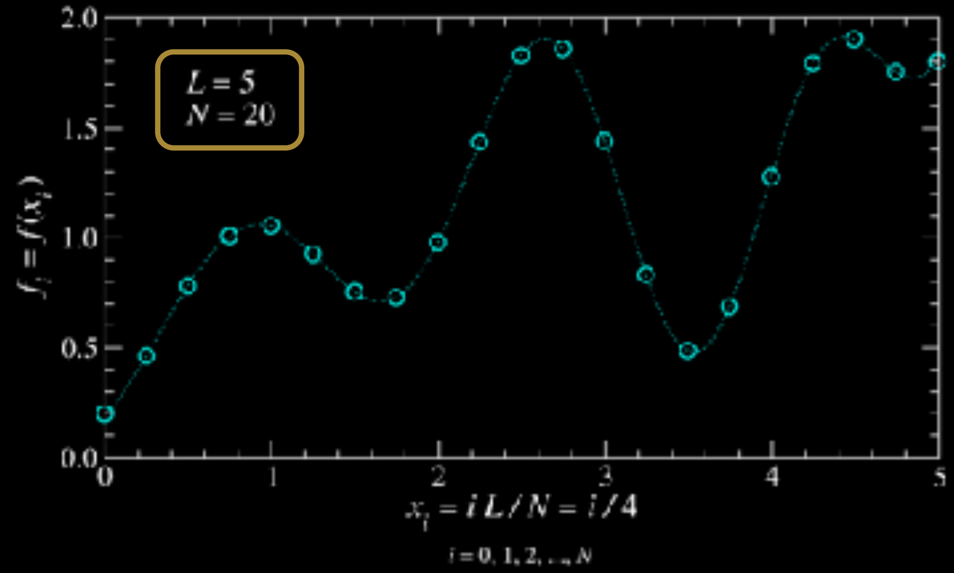

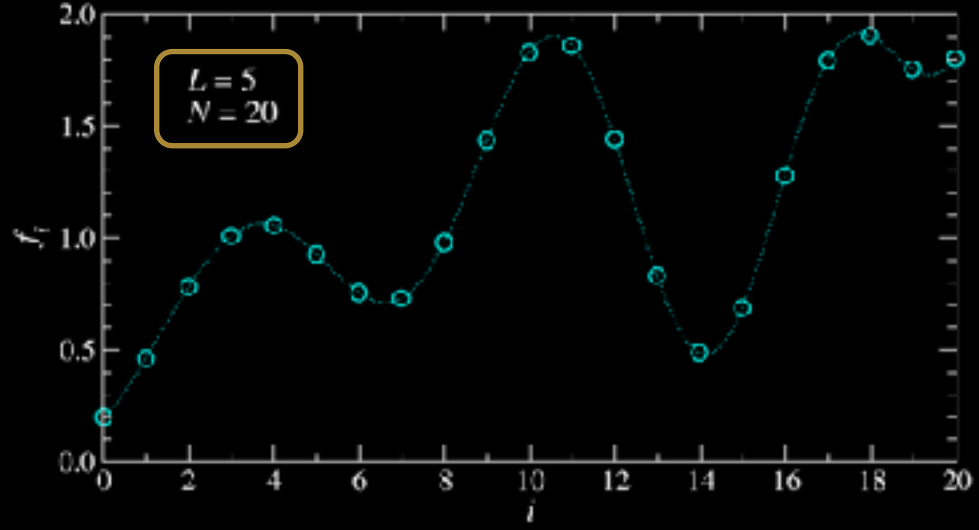

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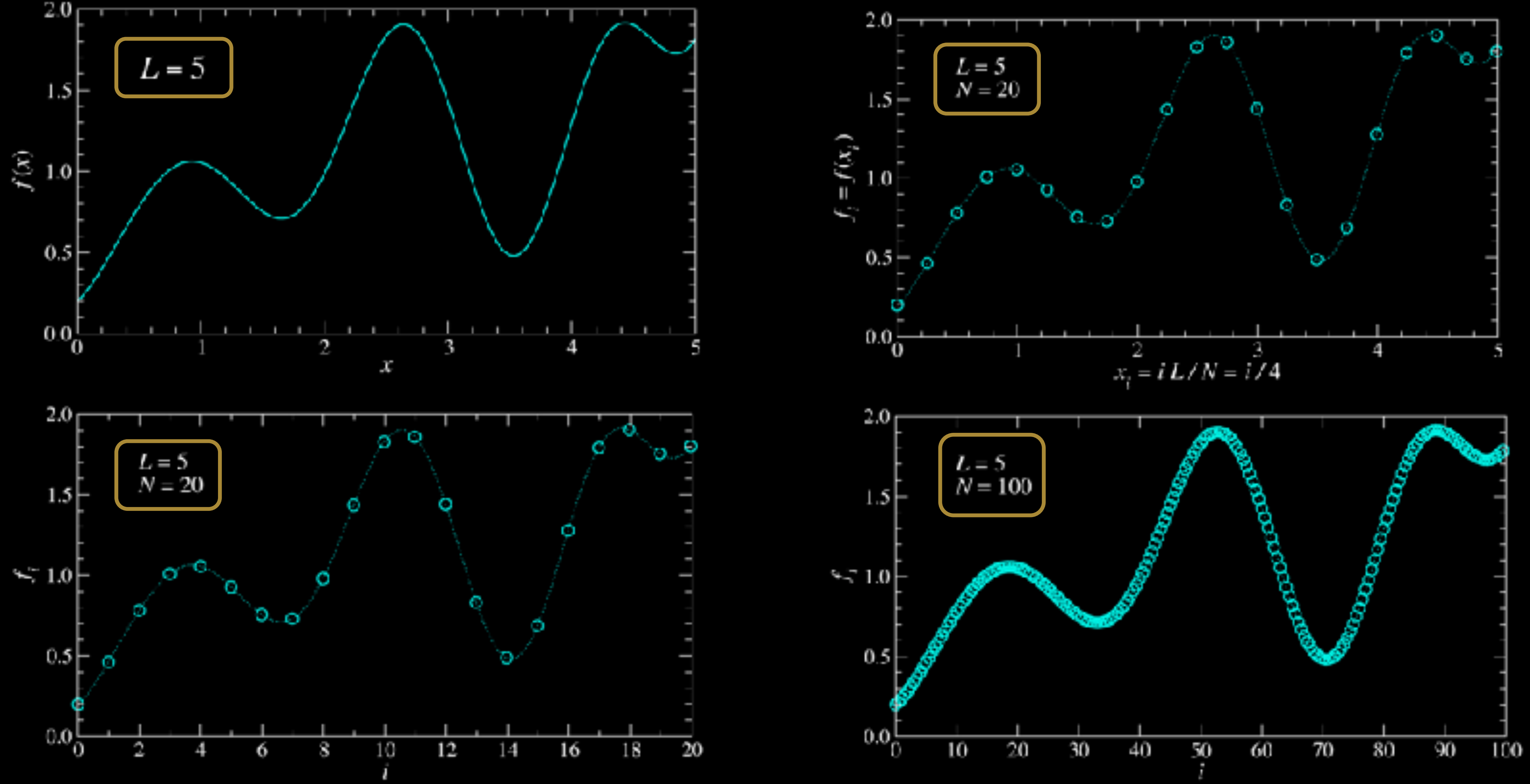
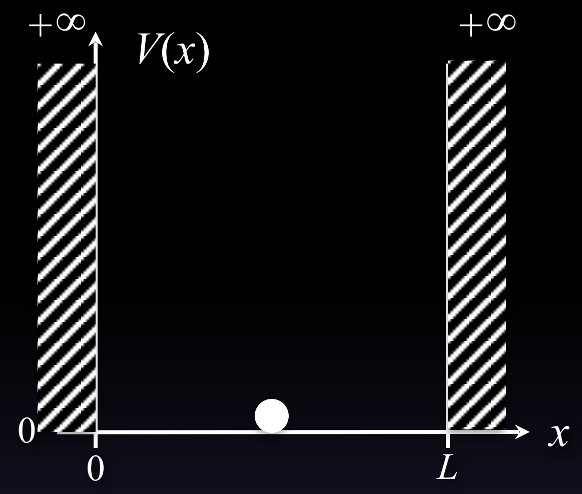


A simple example: 1D particle in a box (infinite potential well)



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$$\left[-\frac{\hbar^2}{2m}\Delta + V(x)\right]\Psi(x) = E\ \Psi(x), \qquad V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty, & \text{otherwise} \end{cases}$$

$$-\Delta\Psi(x) - \frac{2m}{\hbar^2}E\ \Psi(x) \qquad \text{let} \qquad \hbar^2 / 2m = 1$$

discretized

$$-\Delta\Psi(x_i) = E'\ \Psi(x_i), \qquad x_i = \frac{iL}{N} \quad \text{and} \quad i = 0,1,2,\ldots,N$$

$$-\frac{\Psi\left(\frac{(i-1)L}{N}\right) - 2\Psi\left(\frac{iL}{N}\right) + \Psi\left(\frac{(i+1)L}{N}\right)}{\left(\frac{L}{N}\right)^2} = E'\ \Psi\left(\frac{iL}{N}\right)$$

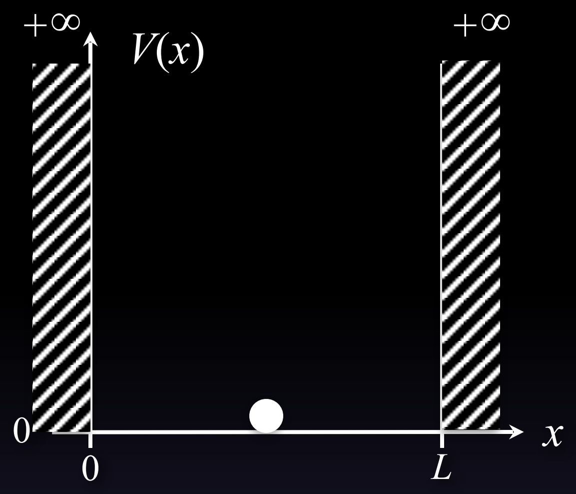
$$-\Psi_{i-1} + 2\Psi_i - \Psi_{i+1} = \tilde{E}\ \Psi_i$$

fixed boundary conditions:

$$\Psi_{-1} = \Psi_{N+1} = 0$$

periodic boundary conditions:

$$\Psi_{-1} = \Psi_{N+1} = -1$$



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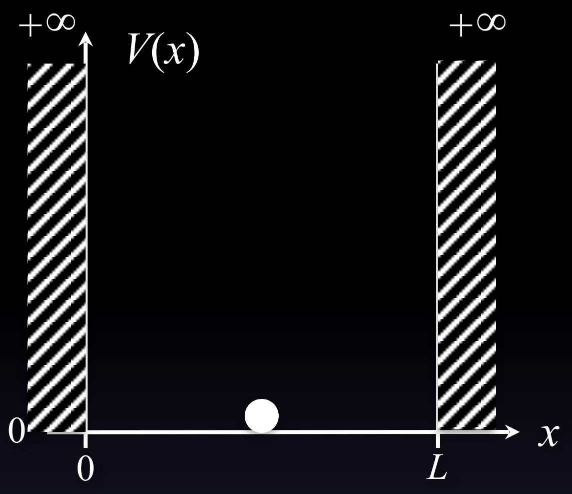

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Matrix to be diagonalized to get E_0:

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & & 0\\ -1 & 2 & -1 & 0 & 0 & & 0\\ 0 & -1 & 2 & -1 & 0 & \cdots & 0\\ 0 & 0 & -1 & 2 & -1 & & 0\\ 0 & 0 & 0 & -1 & 2 & & 0\\ & & \vdots & & & \ddots & \vdots\\ 0 & 0 & 0 & 0 & 0 & \cdots & 2 \end{pmatrix} \begin{pmatrix}\Psi_0\\ \Psi_1\\ \Psi_2\\ \Psi_3\\ \\ \\ \Psi_N\end{pmatrix} = \tilde{E}_0 \begin{pmatrix}\Psi_0\\ \Psi_1\\ \Psi_2\\ \Psi_3\\ \\ \\ \Psi_N\end{pmatrix}$$

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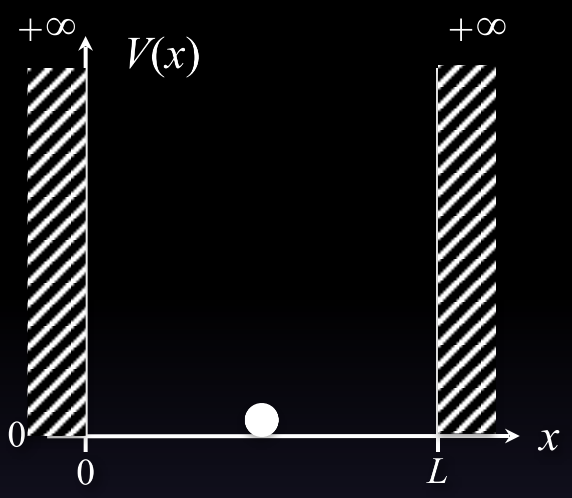

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$$\hat{H} = -\frac{\partial^2}{\partial x^2} \approx -\sum_{j=1}^{N=1}\left(\hat{c}_j^{+}\hat{c}_{j+1} + \hat{c}_{j+1}^{+}\hat{c}_j\right) + 2\sum_{j=1}^{N=1}\hat{c}_j^{+}\hat{c}_j$$

Exact solution exists!

For the 1D particle in the box we get:

$$E_n = \frac{\pi^2}{L^2} n^2, \qquad n = 1,2,\ldots$$

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi\, n}{L} x\right)$$

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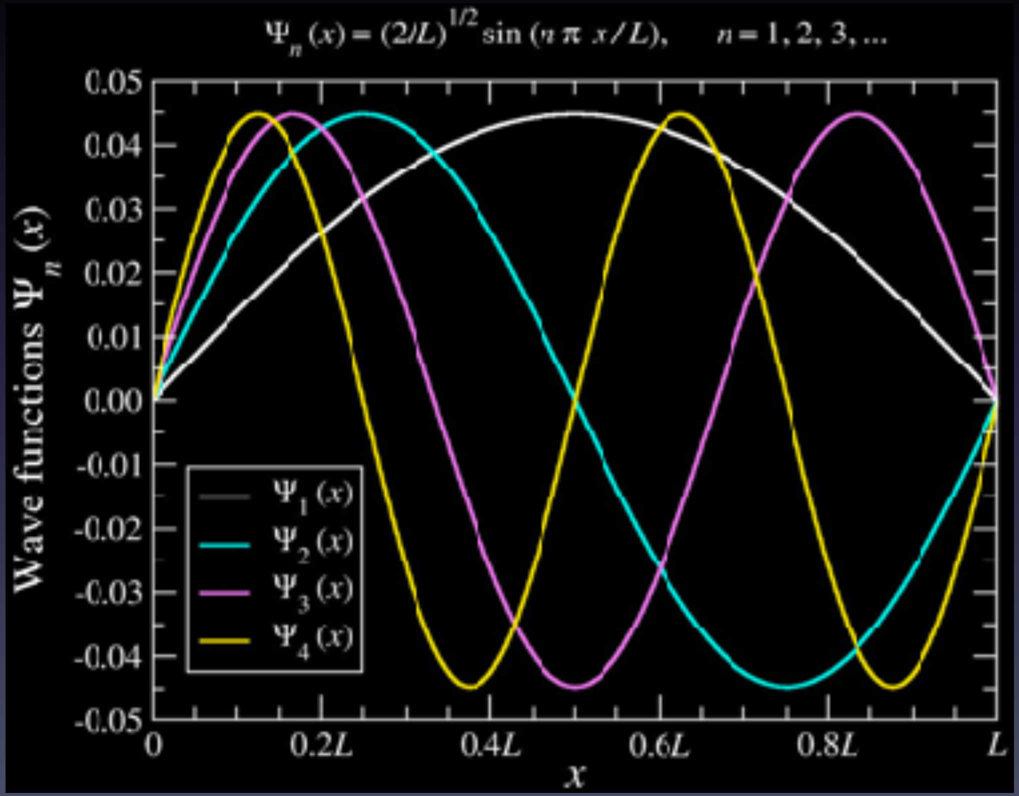

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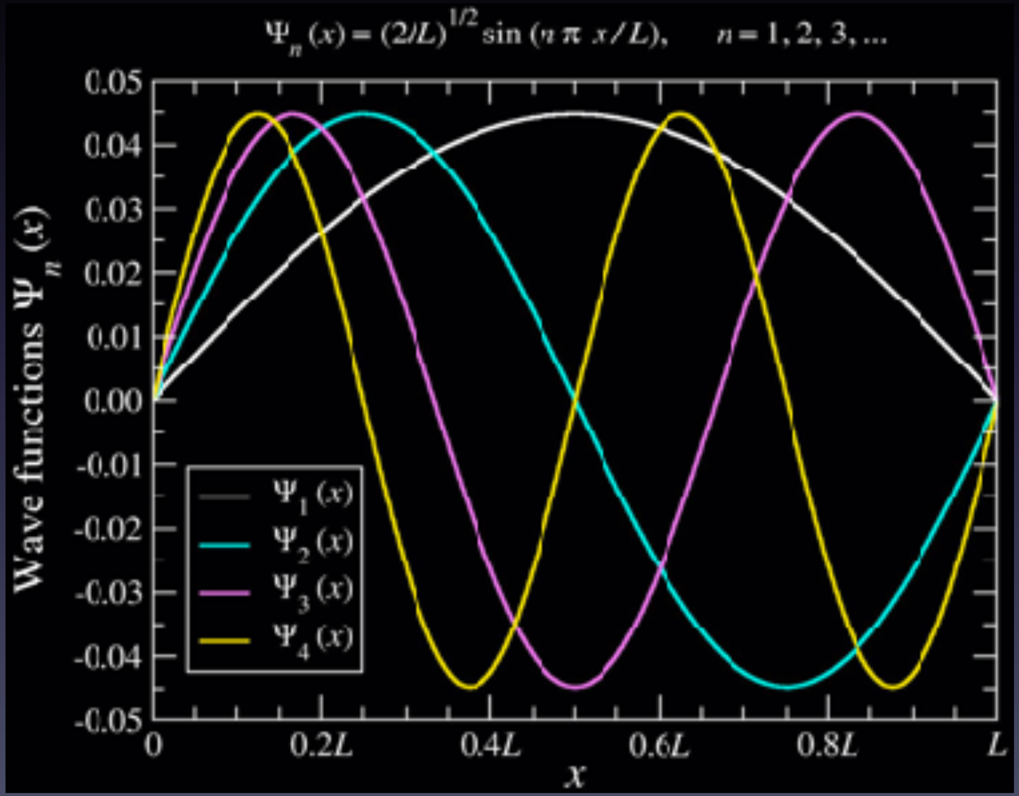
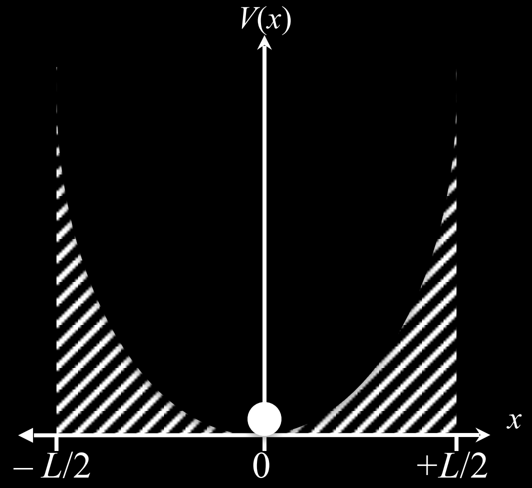


	Relative error $\varepsilon = (E_N^{num} - E_N^{exact}) / E_N^{exact} \times 100\%$			
N	ε_0 [%]	ε_1 [%]	ε_2 [%]	ε_3 [%]
100	1.978	2.002	2.042	2.098
500	0.399	0.400	0.402	0.404
1 000	0.200	0.200	0.200	0.201
5 000	0.040	0.040	0.040	0.040
10 000	0.020	0.020	0.020	0.020
50 000	0.004	0.004	0.004	0.004

Another simple example: Linear Harmonic Oscillator in 1D



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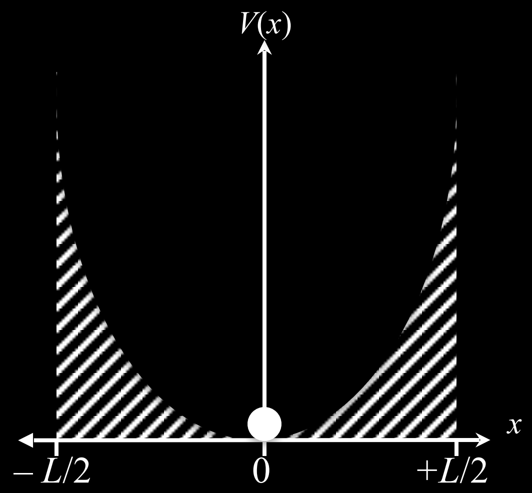
$$-\Delta\Psi(x) + x^2\Psi(x) = 2E'\ \Psi(x)$$

$$-\Delta\Psi(x_i) + (x_i)^2\Psi(x_i) = 2E'\ \Psi(x_i),$$

$$-\frac{\Psi\left(\frac{(i-1)L}{N}\right) - 2\Psi\left(\frac{iL}{N}\right) + \Psi\left(\frac{(i+1)L}{N}\right)}{\left(\frac{L}{N}\right)^2} + \left(\frac{iL}{N}\right)^2\Psi\left(\frac{iL}{N}\right) = 2E'\ \Psi\left(\frac{iL}{N}\right)$$



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$$\hat{H} = -\sum_{i=-N/2}^{N/2}\left(\hat{c}_i^+\hat{c}_{i+1} + \hat{c}_{i+1}^+\hat{c}_i\right) + \sum_{i=-N/2}^{N/2}\left[2\hat{c}_i^+\hat{c}_i + \left(i-\tfrac{L}{2}\right)^2\right] = \sum_{i=0}^{N}\left(\hat{a}_i^+\hat{a}_i + \tfrac{1}{2}\right) \approx -\frac{\partial^2}{\partial x^2} + x^2$$

An exact solution exists:

Hermite polynomials

$$E_n = \left(n + \tfrac{1}{2}\right), \qquad n = 0,1,2,\ldots$$

$$\Psi_n(x) = \frac{1}{\sqrt{2^n n!}} \sqrt{\frac{1}{\sqrt{\pi}}} \exp\left(-\frac{x^2}{2}\right) \underbrace{(-1)^n \exp\left(x^2\right) \frac{\mathrm{d}^n}{\mathrm{d}x^n}\left[\exp\left(-x^2\right)\right]}_{H_n(x)}$$

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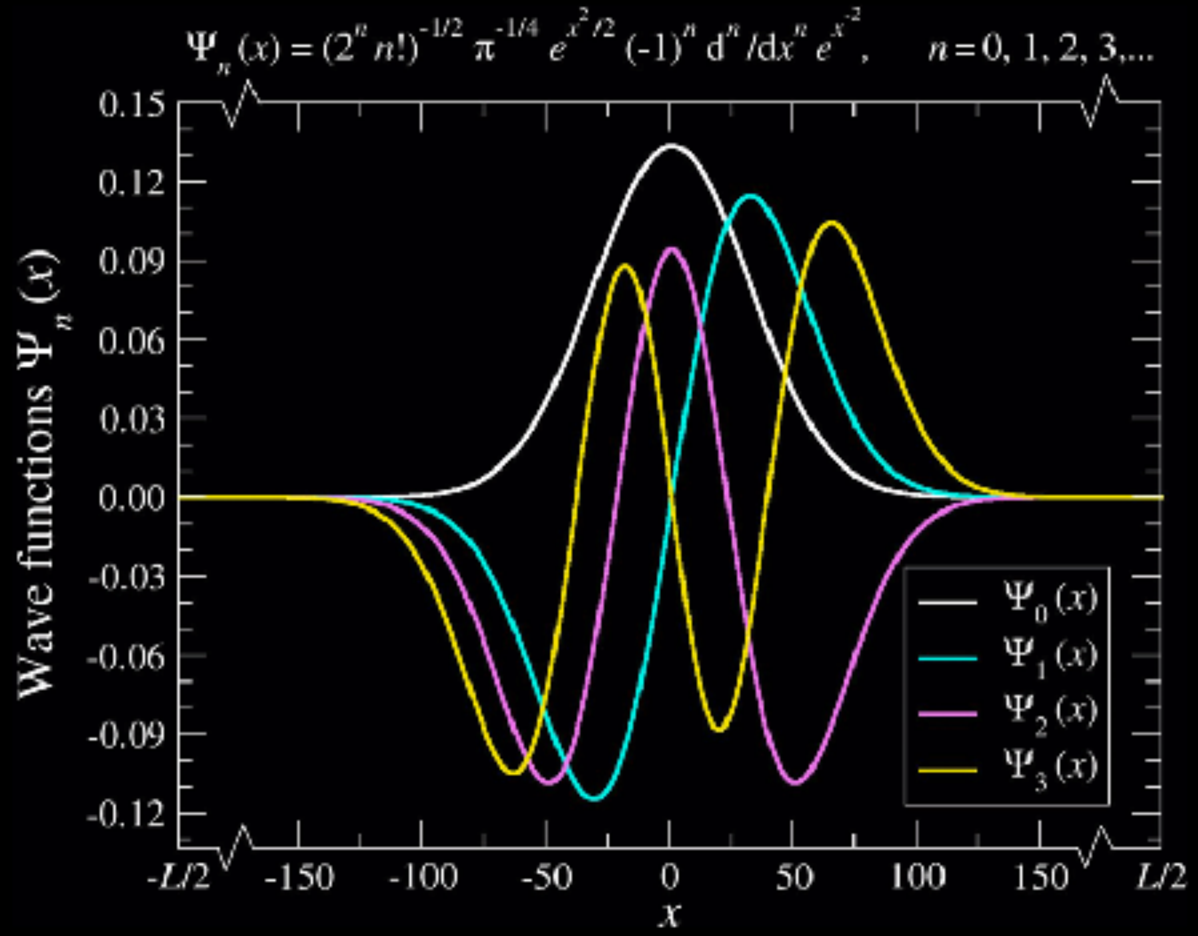

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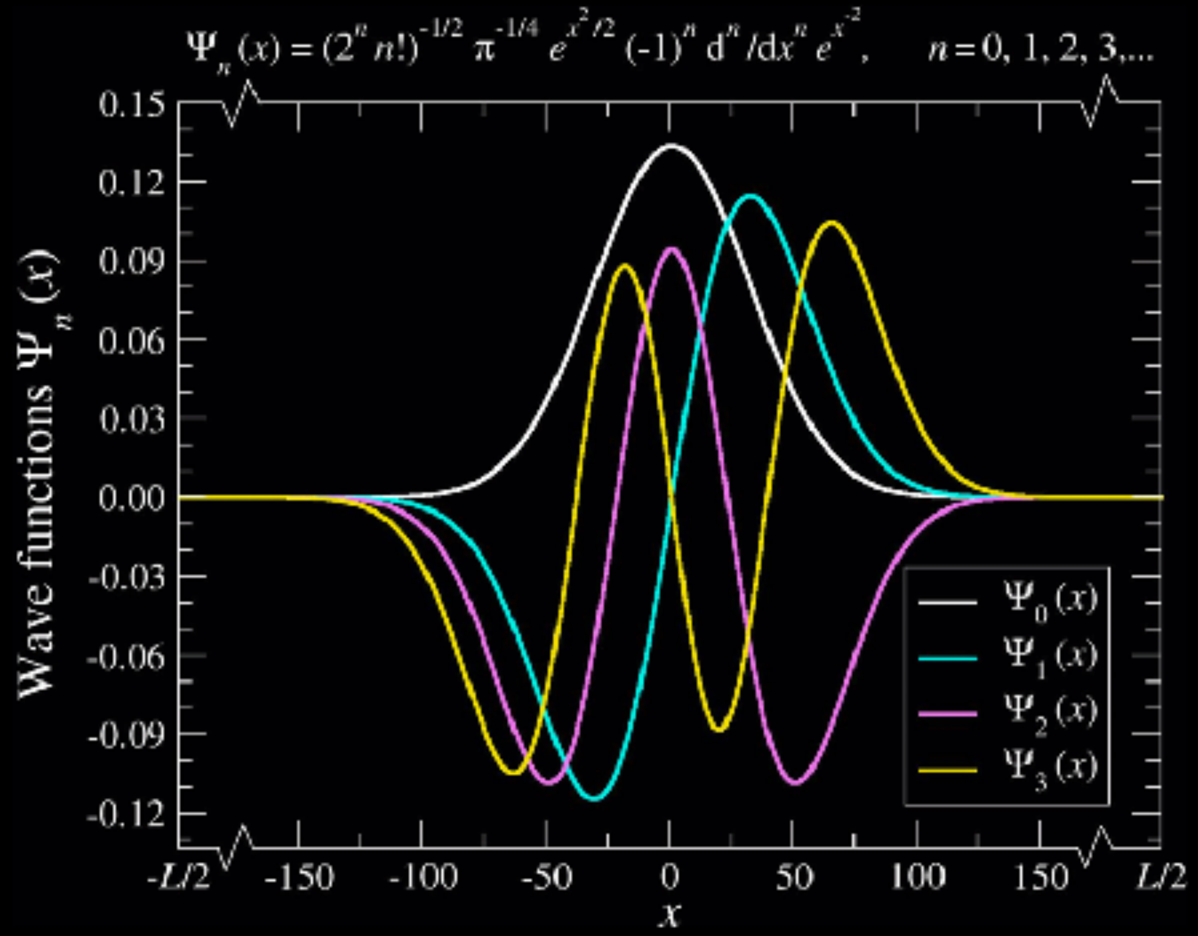

Recall that $\hbar = \omega = m = 1$

	Relative error $\varepsilon = (E_n^{num} - E_n^{exact})/E_n^{exact} \times 100\%$			
N	ε_0	ε_1	ε_2	ε_3
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Numerical efficiency when diagonalizing matrices by DMRG:

- Single-particle problem

- Many-body problem

Numerical efficiency when diagonalizing matrices by DMRG:

- ➢ Single-particle problem

Size	Matrix dimension of Hamiltonian	
N	Exact diagonalization	DMRG
10	10	4
100	100	4
1000	1000	4
10 000	10 000	4

- ➢ Many-body problem

Numerical efficiency when diagonalizing matrices by DMRG:

➢ Single-particle problem

Size	Matrix dimension of Hamiltonian	
N	Exact diagonalization	DMRG
10	10	4
100	100	4
1000	1000	4
10 000	10 000	4

➢ Many-body problem

Lattice size	Estimated memory consumption in a computer		The model
N	Exact diagonalization	DMRG	
10	1 MB	≈ 1 MB	Heisenberg model
100	10^{50} GB	≈ 100 MB	
1000	10^{600} GB	≈ 1 GB	
10	1 GB	< 8 MB	Hubbard model
100	10^{100} GB	≈ 1 GB	
1000	10^{1200} GB	≈ 10 GB	

Schrödinger equation

(for a single particle in 3D)

$$i\hbar\frac{\partial}{\partial t}\left|\Psi\left(\vec{r},t\right)\right\rangle = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\left(\vec{r},t\right)\right]\left|\Psi\left(\vec{r},t\right)\right\rangle$$

Schrödinger equation

(for a single particle in 3D)

$$i\hbar \frac{\partial}{\partial t} \left| \Psi\left(\vec{r}, t\right) \right\rangle = \left[-\frac{\hbar^2}{2m} \nabla^2 + V\left(\vec{r}, t\right) \right] \left| \Psi\left(\vec{r}, t\right) \right\rangle$$

Time-independent Schrödinger equation

(for N particles in 1D)

$$\sum_{j=1}^{N} \left[-\frac{\hbar^2}{2m_j} \frac{\partial^2}{\partial x_j^2} + V(x_1, x_2, \ldots, x_N) \right] \left| \Psi_n(x_1, x_2, \ldots, x_N) \right\rangle = E_n \left| \Psi_n(x_1, x_2, \ldots, x_N) \right\rangle$$

Schrödinger equation

(for a single particle in 3D)

$$i\hbar\frac{\partial}{\partial t}\left|\Psi\left(\vec{r},t\right)\right\rangle = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\left(\vec{r},t\right)\right]\left|\Psi\left(\vec{r},t\right)\right\rangle$$

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Time-independent Schrödinger equation in second quantization

(for N interacting particles in 1D)

$$\underbrace{\left[-t\sum_{j=1}^{N-1}\left(c_j^+c_{j+1} + c_{j+1}^+c_j\right) - \sum_{j=1}^{N} V_j c_j^+ c_j - U\sum_{j=1}^{N-1} c_j^+c_jc_{j+1}^+c_{j+1}\right]}_{H}\left|\phi_n\right\rangle = E_n\left|\phi_n\right\rangle$$

Schrödinger equation

(for a single particle in 3D)

$$i\hbar\frac{\partial}{\partial t}\left|\Psi\left(\vec{r},t\right)\right\rangle = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\left(\vec{r},t\right)\right]\left|\Psi\left(\vec{r},t\right)\right\rangle$$

Time-independent Schrödinger equation

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Time-independent Schrödinger equation in second quantization

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$$H\left|\phi_n\right\rangle = E_n\left|\phi_n\right\rangle$$

Solving the Schrödinger equation means finding E_n and $\left|\phi_n\right\rangle$ (typically by diagonalizing the Hamiltonian).

How to obtain <u>an entangled state</u> analytically?

$$H = -J\left(S_1^x \otimes S_2^x + S_1^y \otimes S_2^y + S_1^z \otimes S_2^z\right) = \begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & J & -2J & 0 \\ 0 & -2J & J & 0 \\ 0 & 0 & 0 & -J \end{pmatrix}$$

How to obtain an entangled state analytically?

$$H = -J\left(S_1^x \otimes S_2^x + S_1^y \otimes S_2^y + S_1^z \otimes S_2^z\right) = \begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & J & -2J & 0 \\ 0 & -2J & J & 0 \\ 0 & 0 & 0 & -J \end{pmatrix}$$

Diagonalize the 4×4 Hamiltonian matrix

$$H\left|\phi_n\right\rangle = E_n\left|\phi_n\right\rangle, \quad n = 0,1,2,3$$

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Diagonalize the 4×4 Hamiltonian matrix

$$H\left|\phi_n\right\rangle = E_n\left|\phi_n\right\rangle, \qquad n = 0,1,2,3$$

$$|\phi_0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad |\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix},$$

Result: $$E = \begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & -J & 0 & 0 \\ 0 & 0 & -J & 0 \\ 0 & 0 & 0 & 3J \end{pmatrix}$$

$$|\phi_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \qquad |\phi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

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$$|\phi_n\rangle = \sum_{i=\uparrow}^{\downarrow}\sum_{j=\uparrow}^{\downarrow}\phi_{ij}|ij\rangle = \phi^{(n)}_{\uparrow\uparrow}|\uparrow\uparrow\rangle + \phi^{(n)}_{\uparrow\downarrow}|\uparrow\downarrow\rangle + \phi^{(n)}_{\downarrow\uparrow}|\downarrow\uparrow\rangle + \phi^{(n)}_{\downarrow\downarrow}|\downarrow\downarrow\rangle = \phi^{(n)}_{\uparrow\uparrow}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \phi^{(n)}_{\uparrow\downarrow}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \phi^{(n)}_{\downarrow\uparrow}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + \phi^{(n)}_{\downarrow\downarrow}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

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Diagonalize the 4×4 Hamiltonian matrix

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Result: $E = \begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & -J & 0 & 0 \\ 0 & 0 & -J & 0 \\ 0 & 0 & 0 & 3J \end{pmatrix}$

$$|\phi_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \qquad |\phi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle$$

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Diagonalize the 4×4 Hamiltonian matrix

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maximally entangled states

Result: $E = \begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & -J & 0 & 0 \\ 0 & 0 & -J & 0 \\ 0 & 0 & 0 & 3J \end{pmatrix}$

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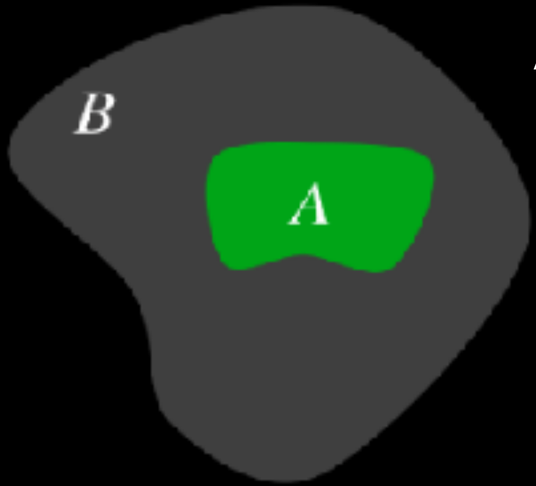
A measure of entanglement: Entanglement entropy

Validity for the Tensor Networks

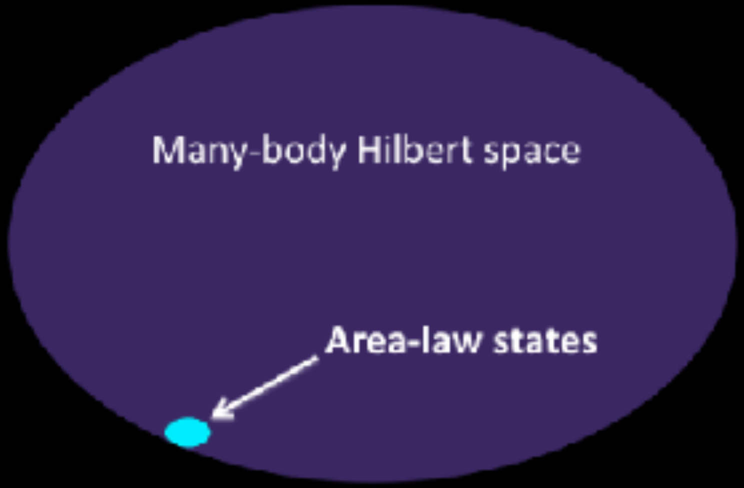
A measure of entanglement: Entanglement entropy

Validity for the Tensor Networks

Area law



$$S \sim \partial A$$



A measure of entanglement: Entanglement entropy

Validity for the Tensor Networks

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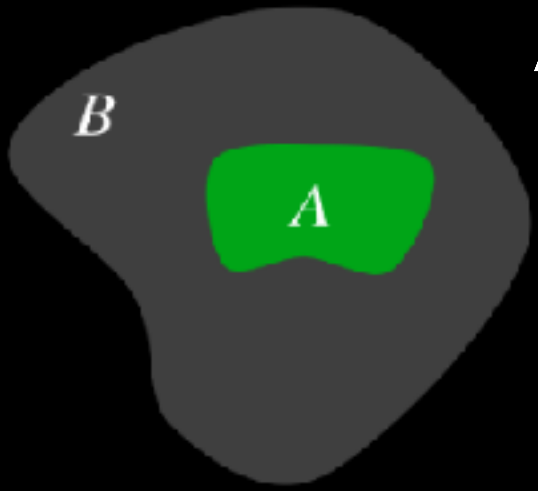

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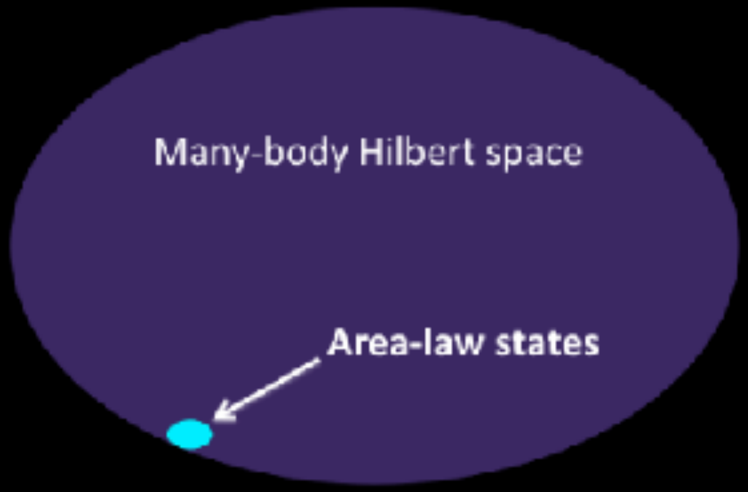

$$|\psi_0(A,B)\rangle = \sum_A \sum_B \psi_{AB} |A\rangle \otimes |B\rangle = \sum_A \sum_B \sum_\xi U_{A\xi} d_\xi V^T_{\xi B} |A\rangle \otimes |B\rangle = \sum_\xi d_\xi |\xi\rangle_A |\xi\rangle_B$$

A measure of entanglement: Entanglement entropy

Validity for the Tensor Networks

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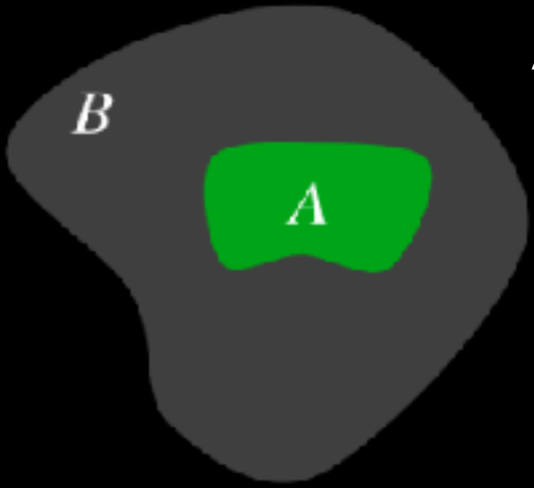

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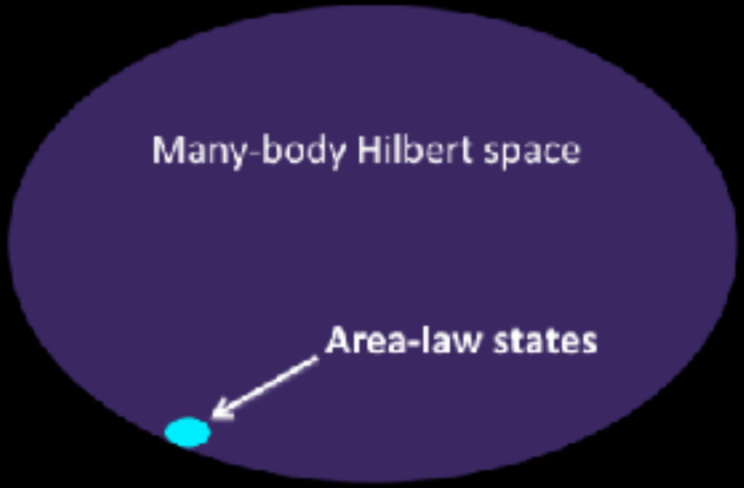

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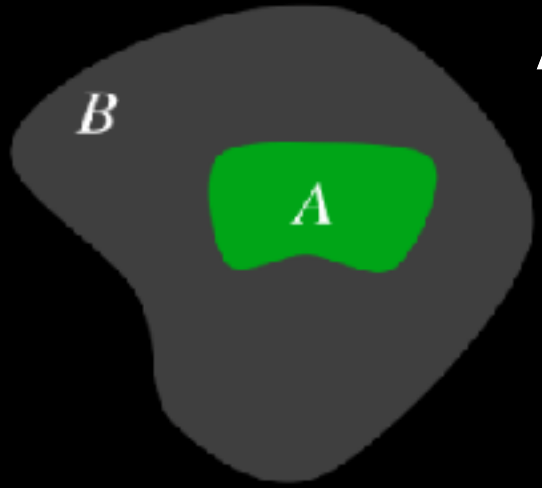
$$\rho'_A = Tr_B \Big\{ |\psi_0(A,B)\rangle \langle \psi_0(A,B)| \Big\}$$

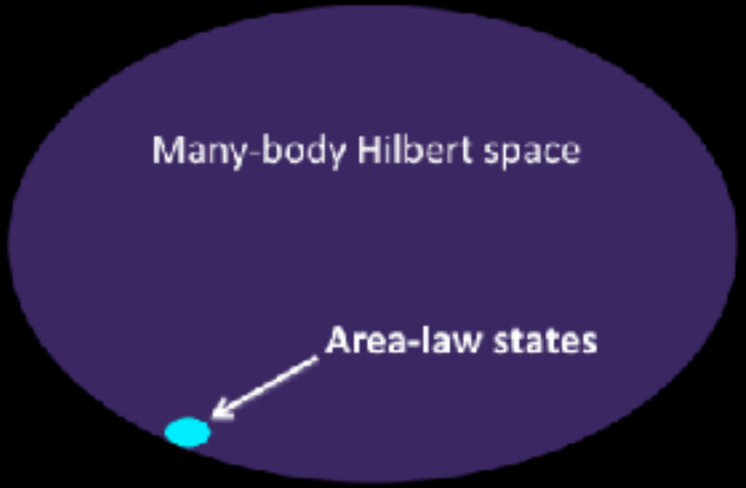
A measure of entanglement: Entanglement entropy

Validity for the Tensor Networks

Area law



$S \sim \partial A$



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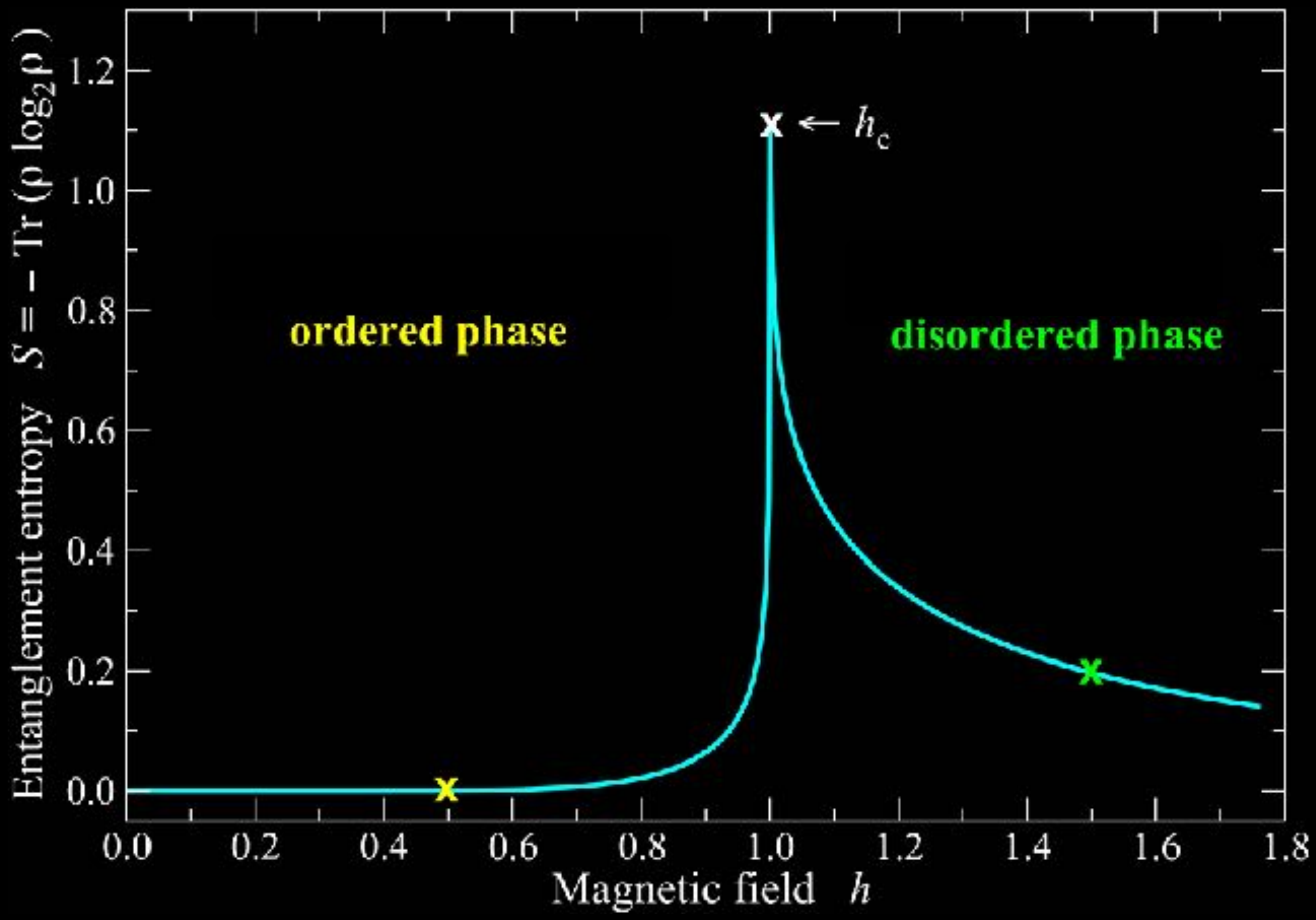
$$\rho'_A = Tr_B \left\{ |\psi_0(A,B)\rangle \langle \psi_0(A,B)| \right\} \qquad S = -\,\mathrm{Tr}\,\left(\rho'_A \log_2 \rho'_A\right) = -\sum_\xi d_\xi^2 \log_2 d_\xi^2$$

Entanglement entropy for a quantum spin system $S = -\mathrm{Tr}\left(\rho' \log_2 \rho'\right)$



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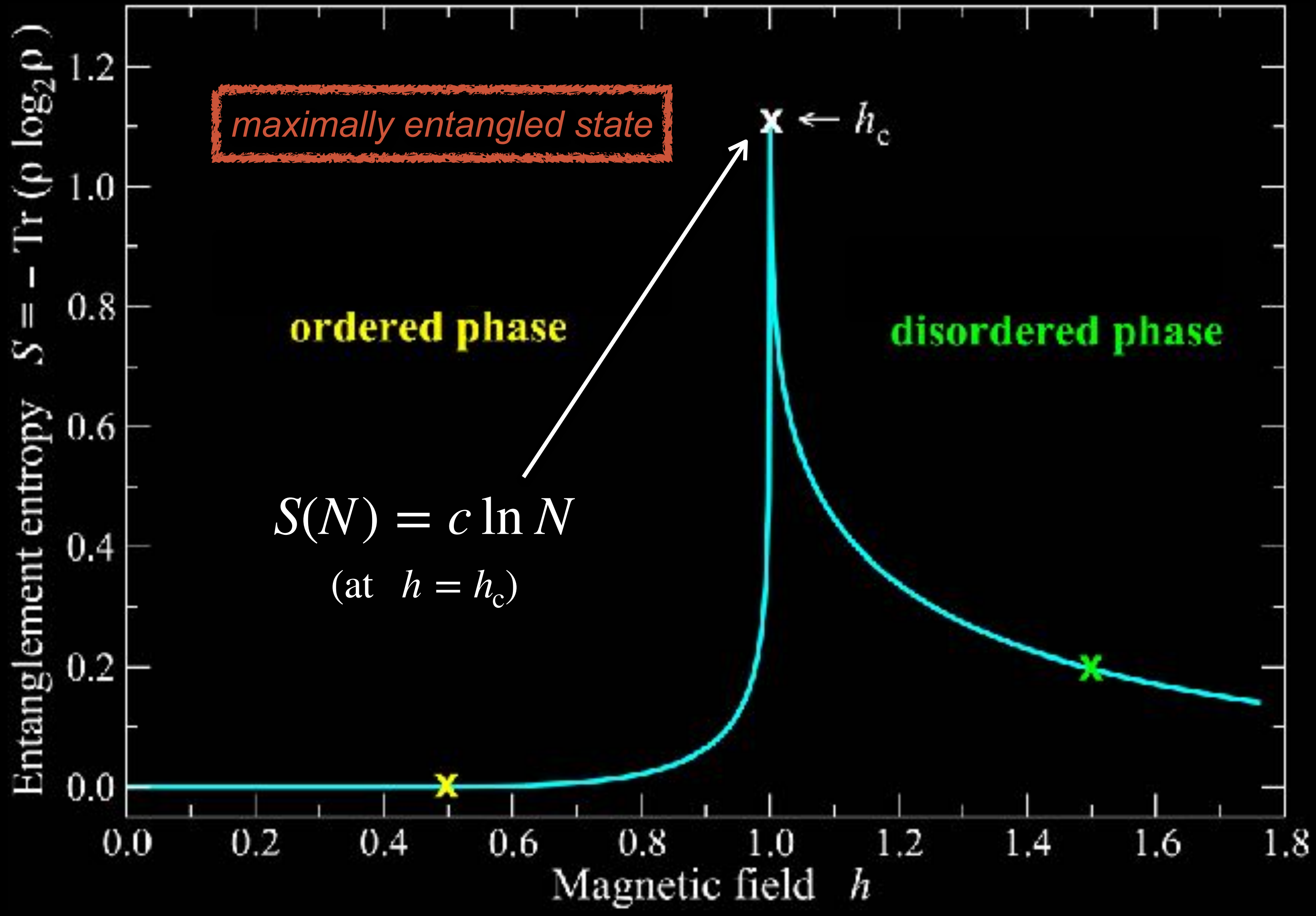
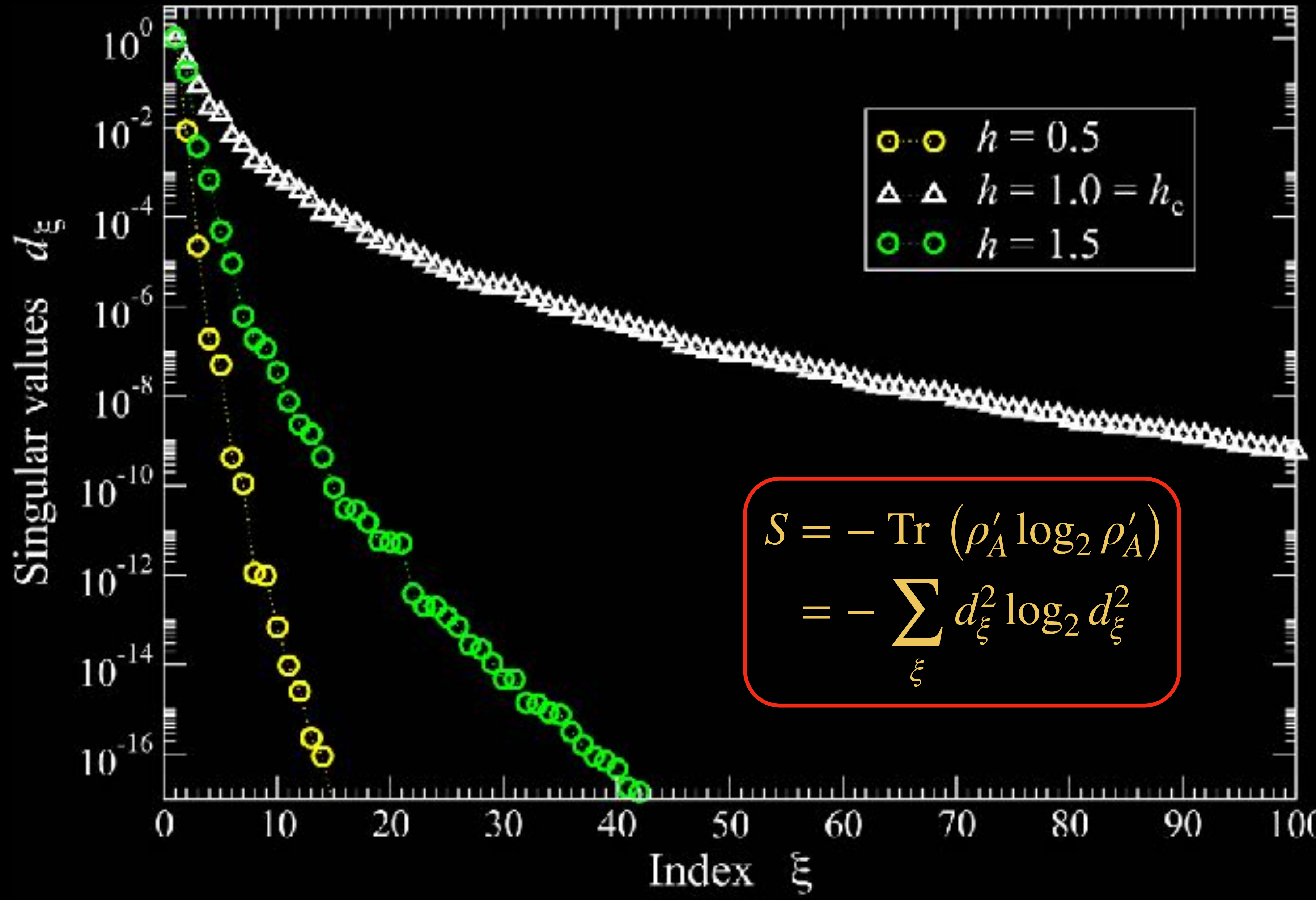


Decay of the singular values (Schmidt coefficients) d_ξ



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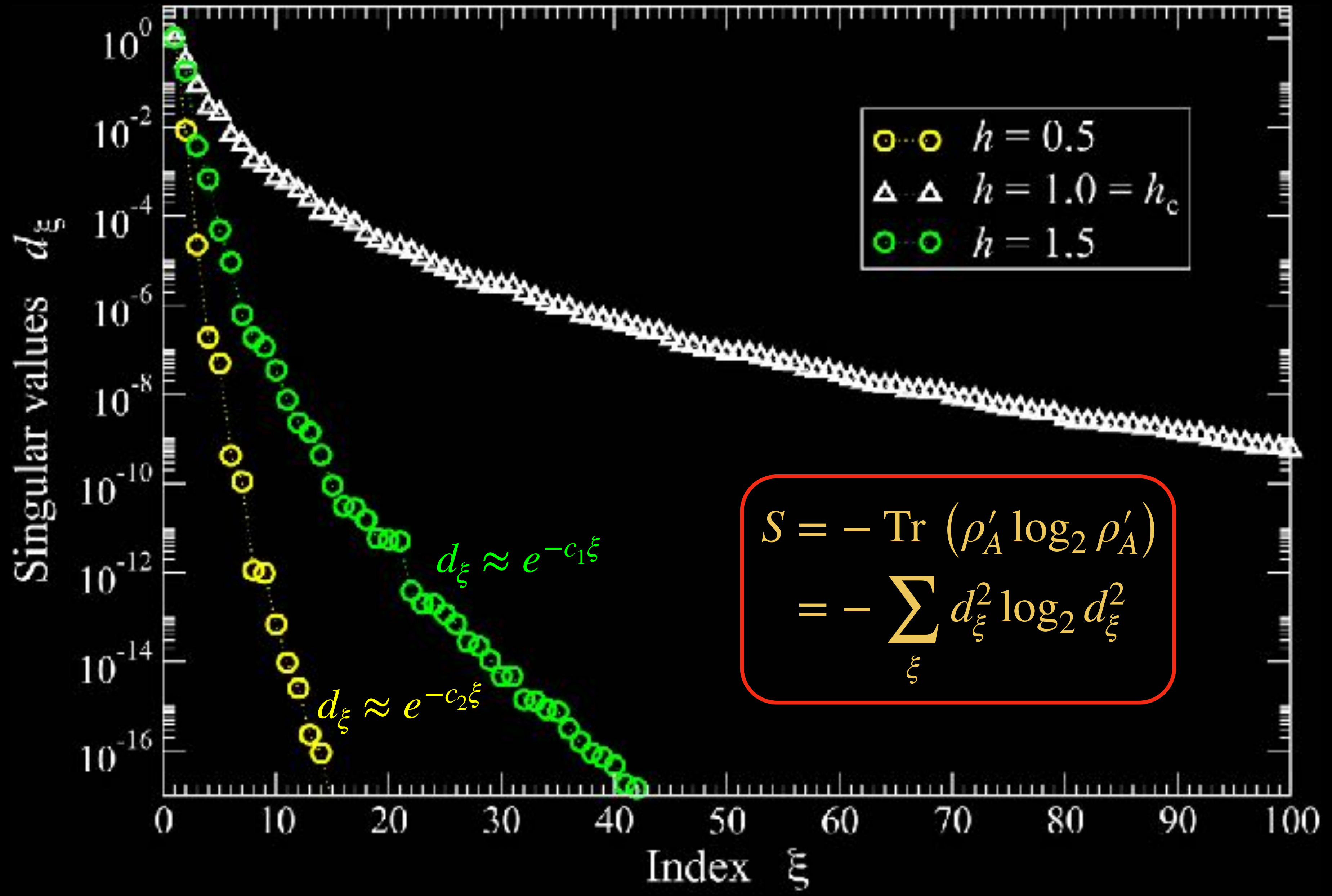

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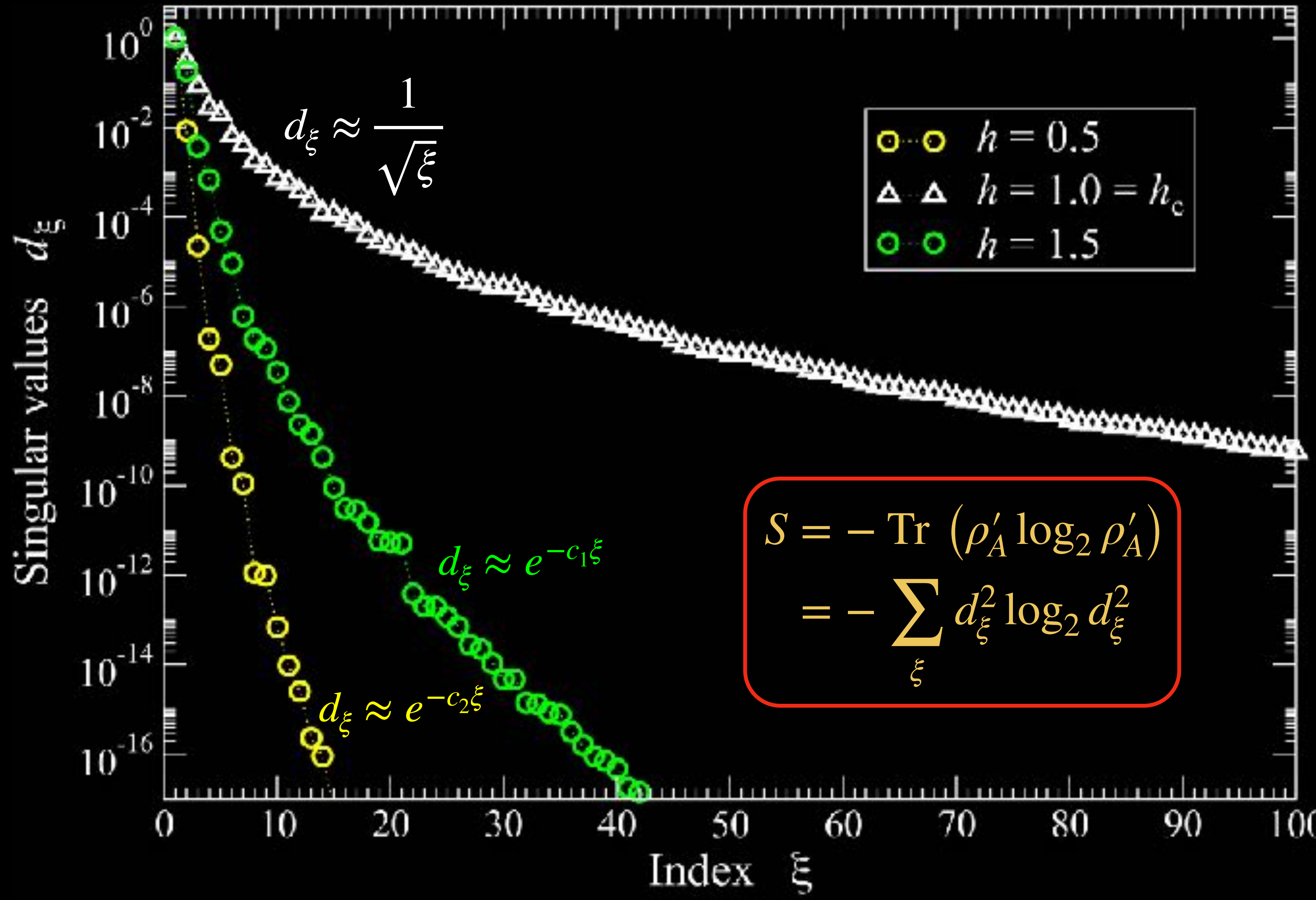

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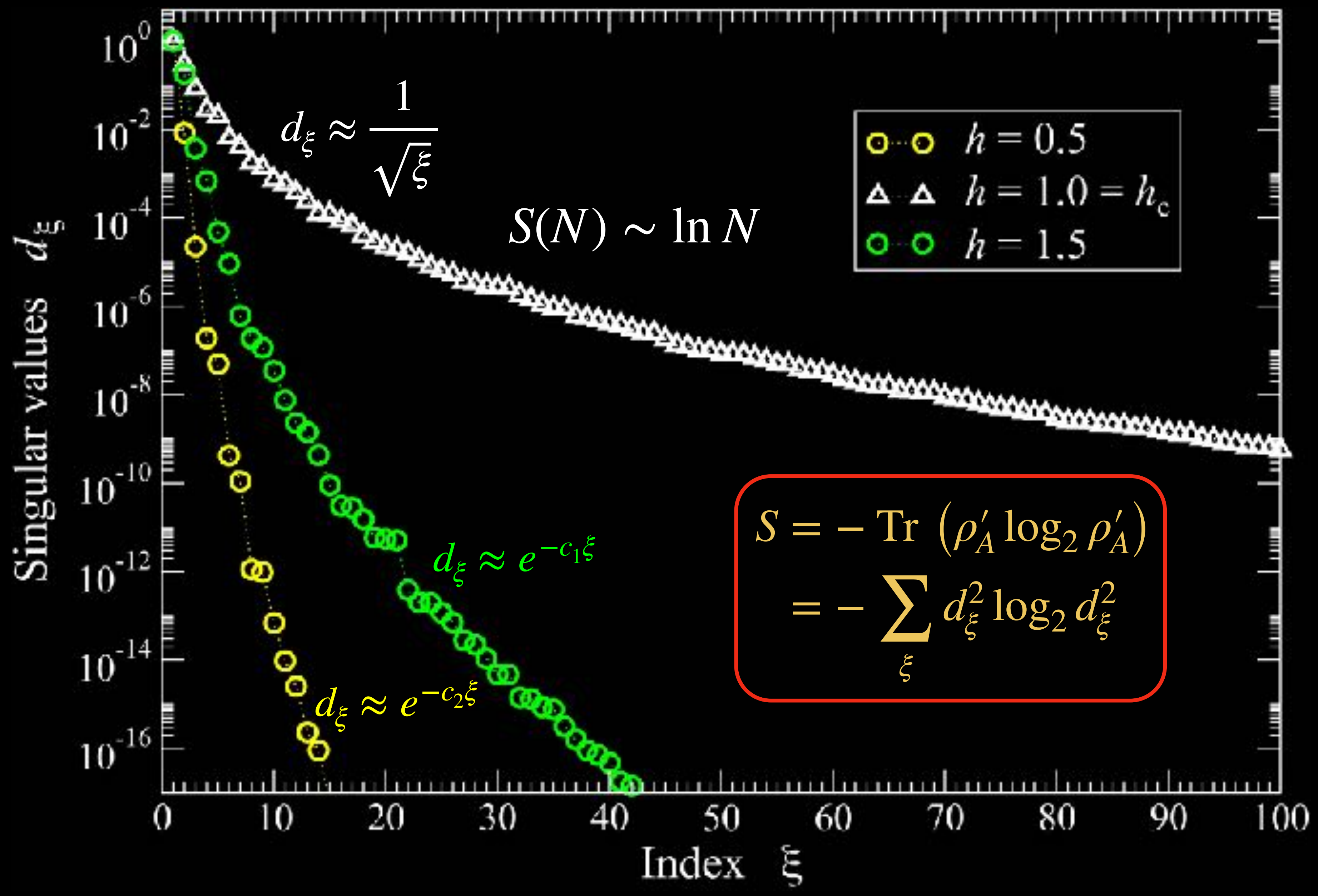
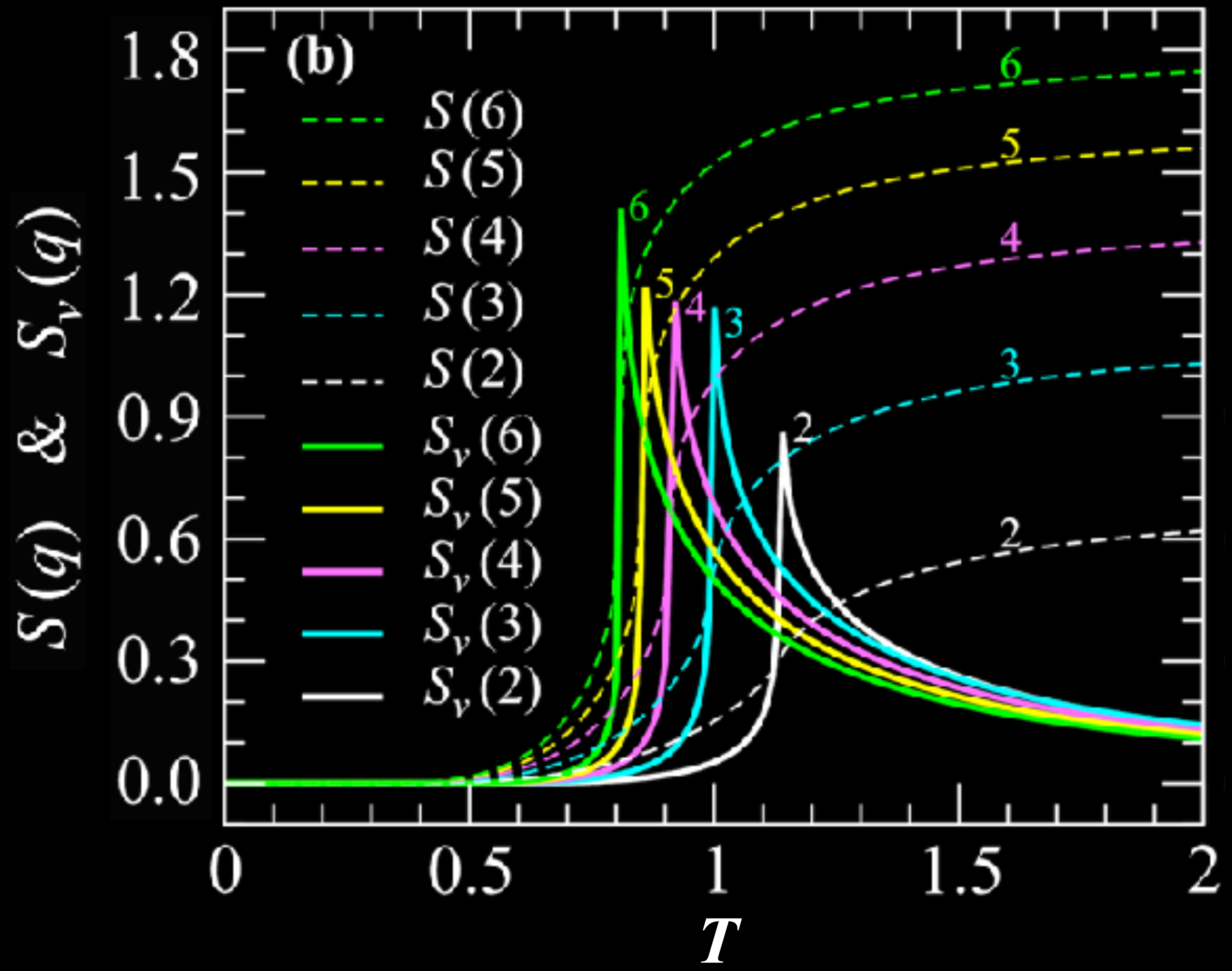
$$= -\sum_{\xi} d_\xi^2 \log_2 d_\xi^2$$

Decay of the singular values (Schmidt coefficients) d_ξ



Comparison between the thermodynamic entropy and entanglement entropy

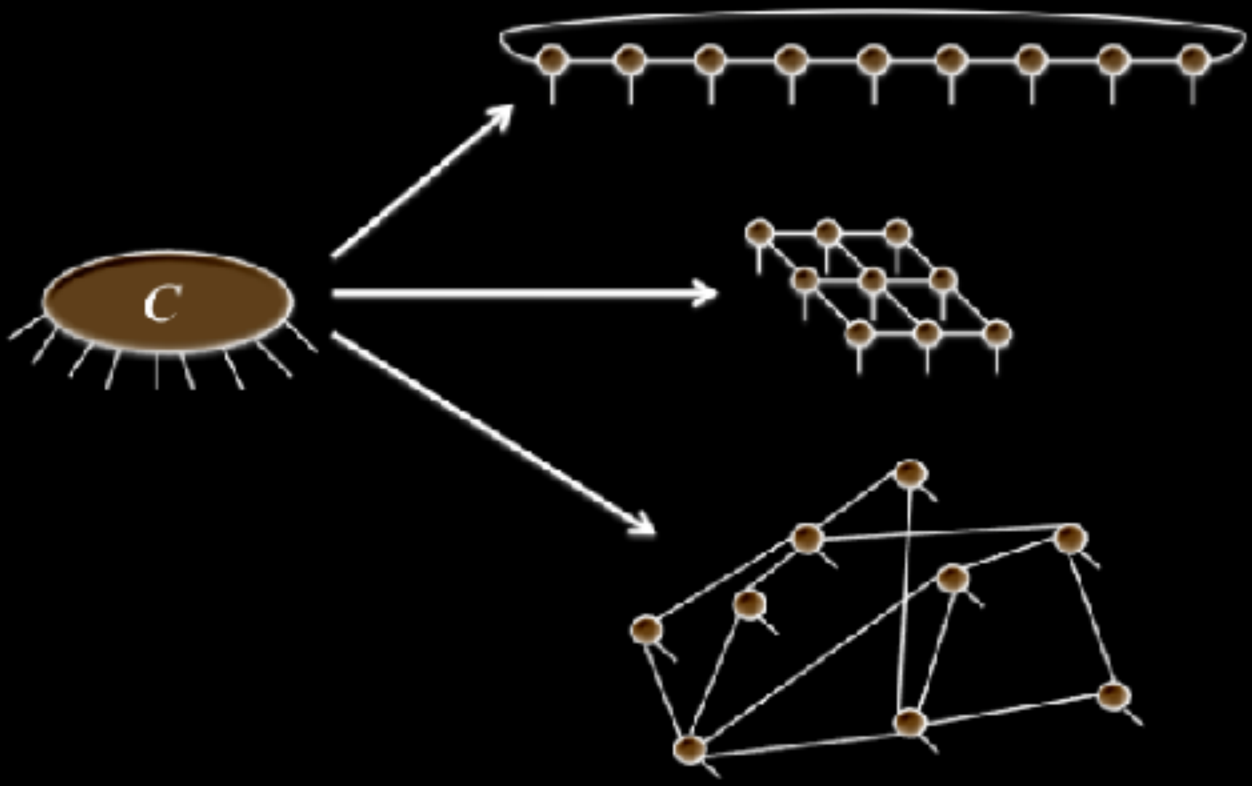


Matrix Product State

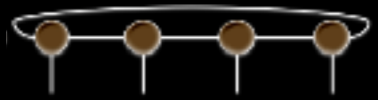
SVD and Entanglement

Tensor Network is a Tensor Product State

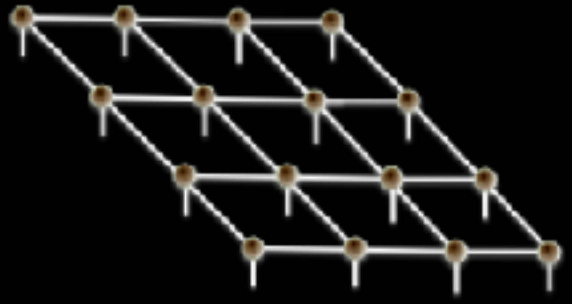
(and it's like playing a Tetris game...)

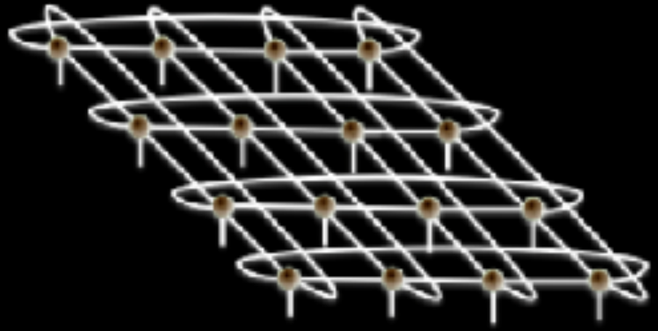


Tensor Network is a Tensor Product State

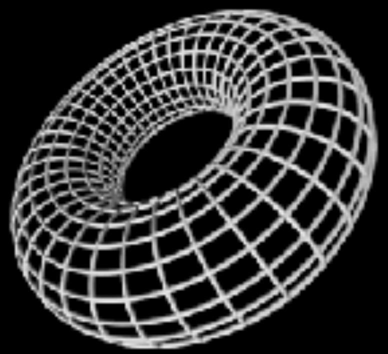


1D state $|\phi\rangle$





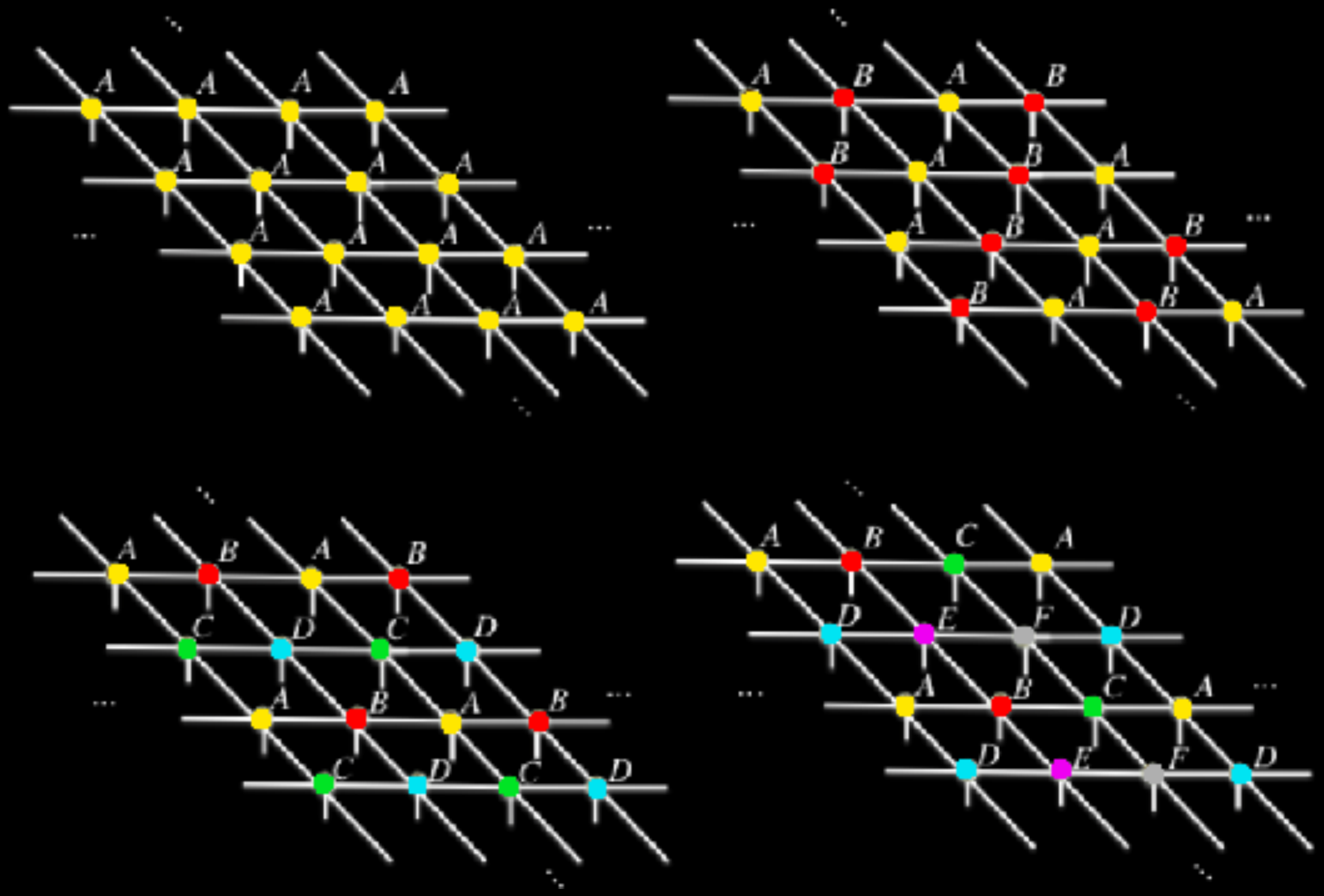
2D state $|\phi\rangle$



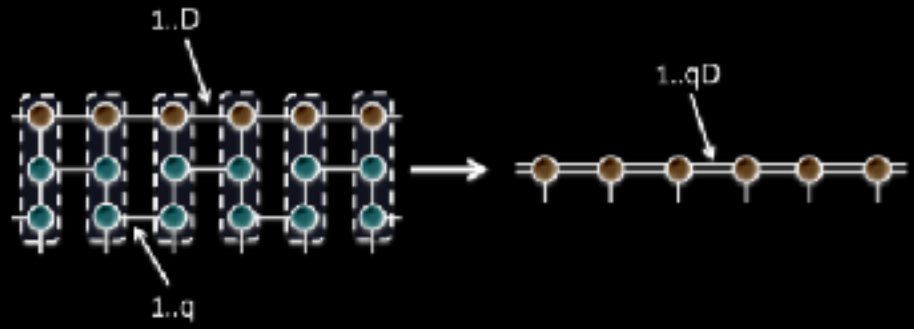
For open/fixed boundary conditions

For periodic boundary conditions (it is a torus!)

Tensor Network is a Tensor Product State

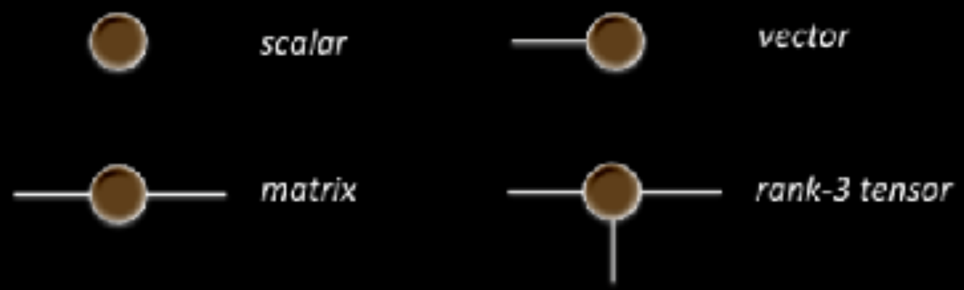


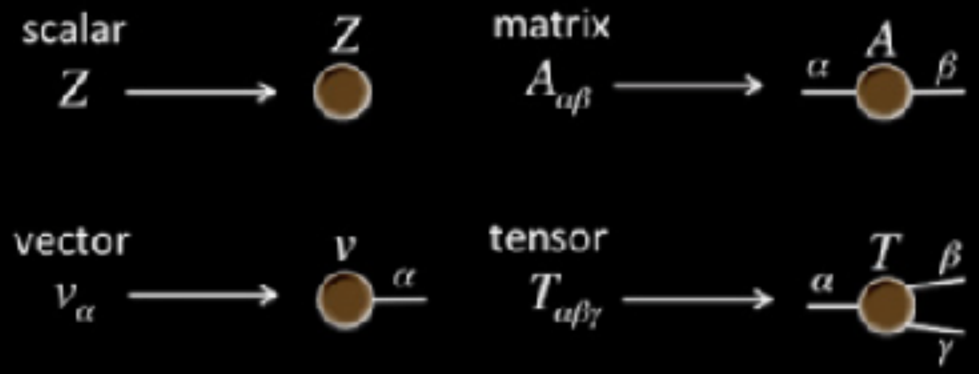
If studying quantum (topological) phases



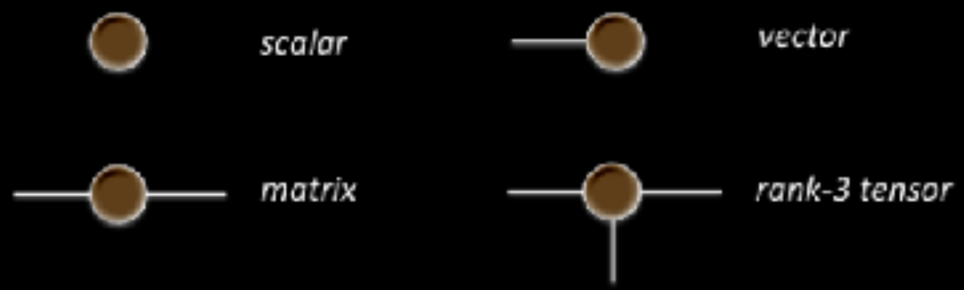
(imaginary) time evolution

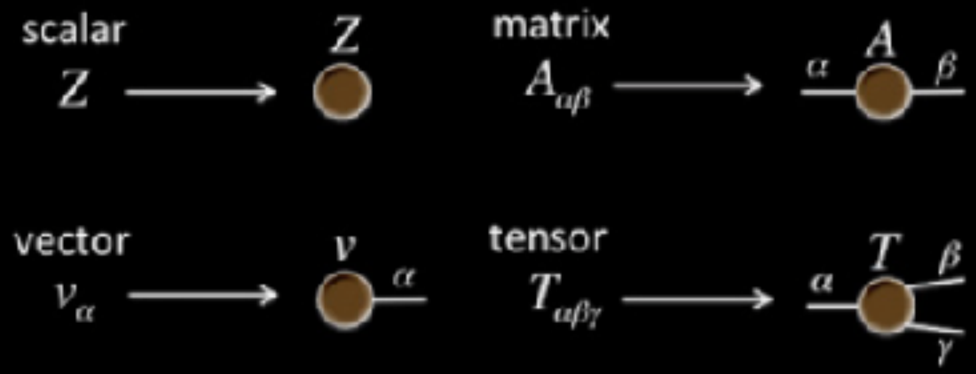
Tensor Network is a Tensor Product State



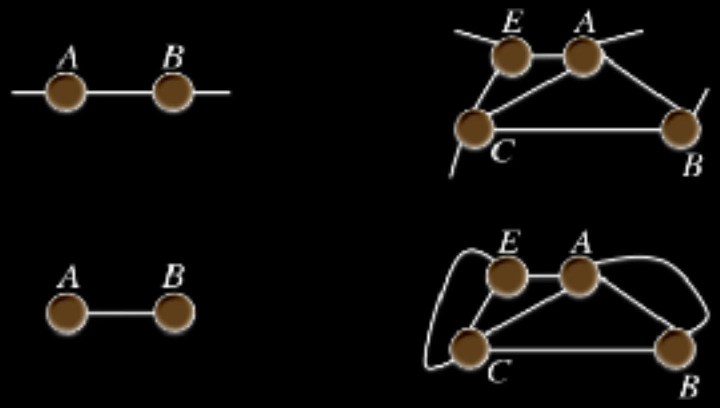


Tensor Network is a Tensor Product State

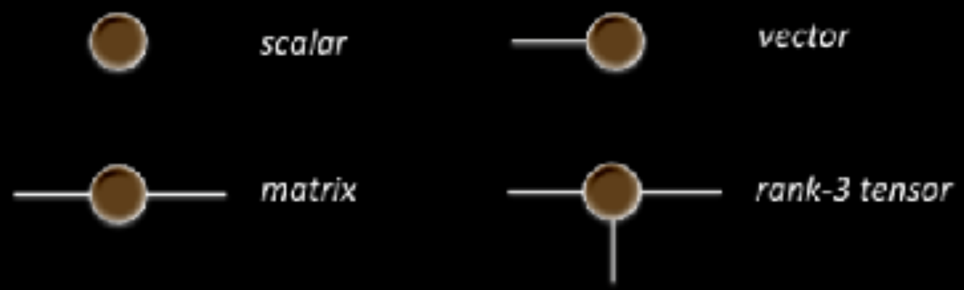


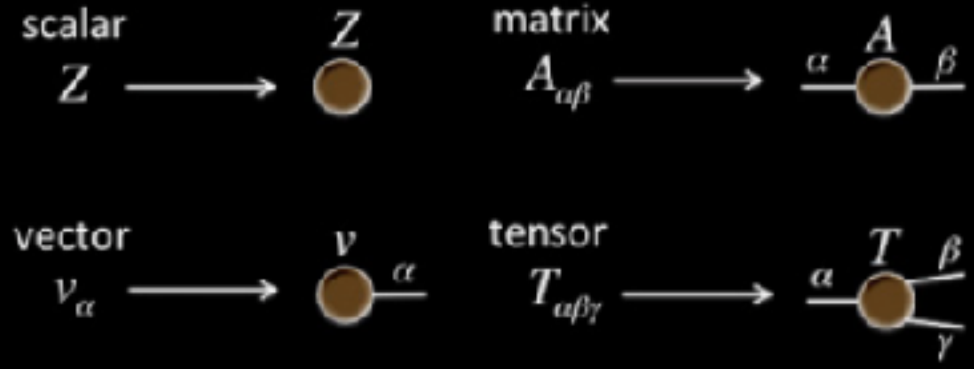


$$\sum_j A_{ij}B_{jk} = D_{ik}$$



Tensor Network is a Tensor Product State





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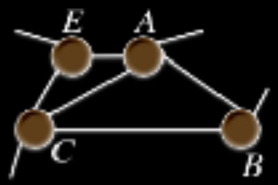
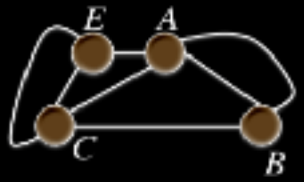
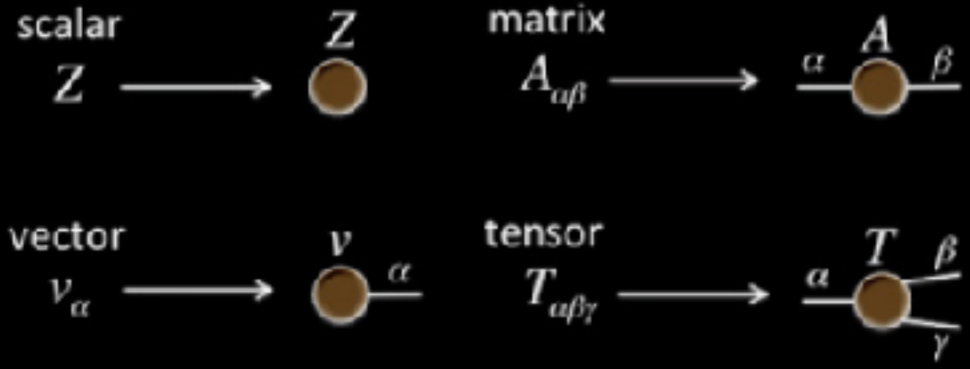




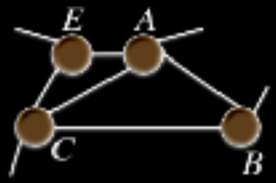
$$\sum_i A_i B_i = \langle A | B \rangle = D$$

Tensor Network is a Tensor Product State

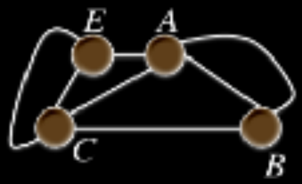


$$\sum_j A_{ij}B_{jk} = D_{ik}$$

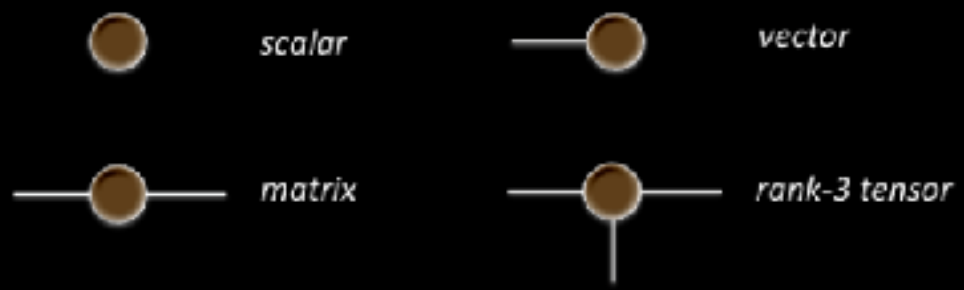
$$\sum_{ikmn} A_{ikjl}B_{ipm}C_{qmkn}E_{lnr} = D_{jpqr}$$

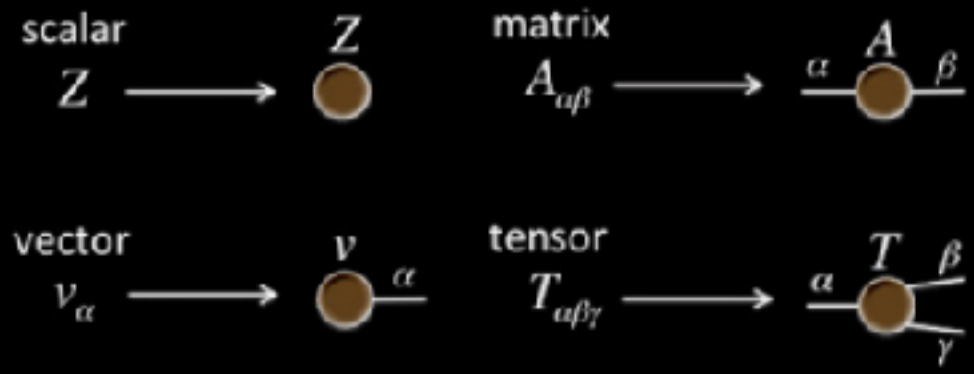


$$\sum_i A_iB_i = \langle A \,|\, B\rangle = D$$



Tensor Network is a Tensor Product State





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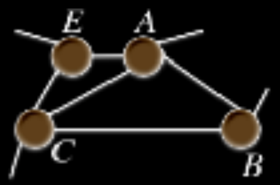

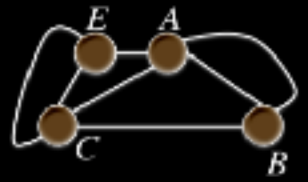

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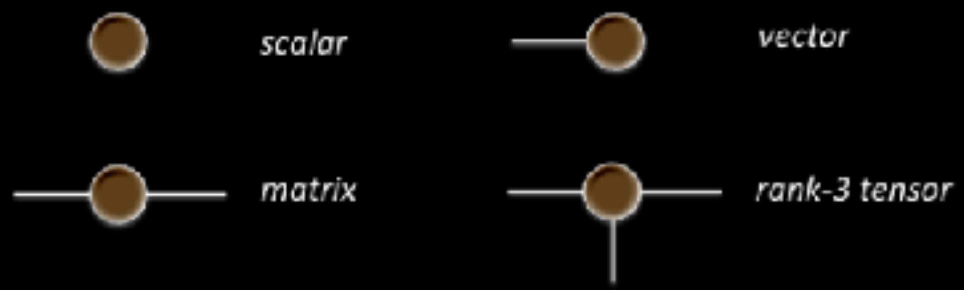
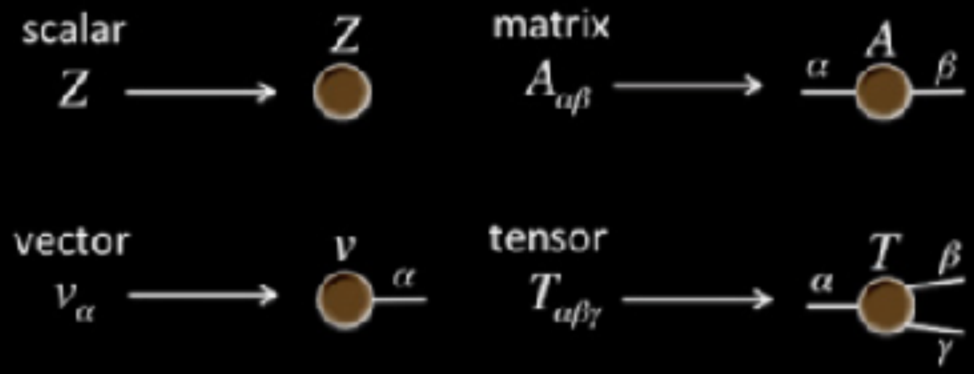
$$\sum_{ijklmnr} A_{ijkl}B_{ijm}C_{kmnr}E_{lknr} = D$$

Tensor Network is a Tensor Product State





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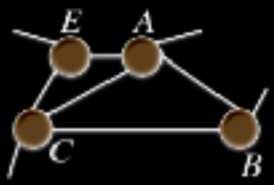

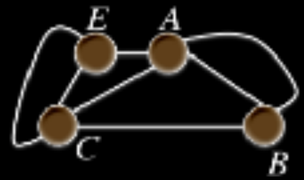

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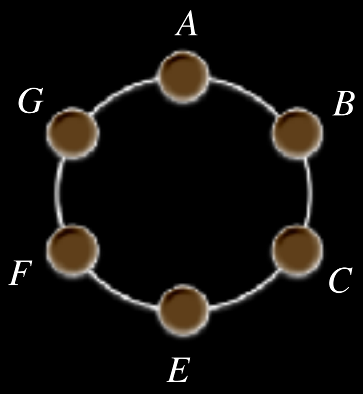

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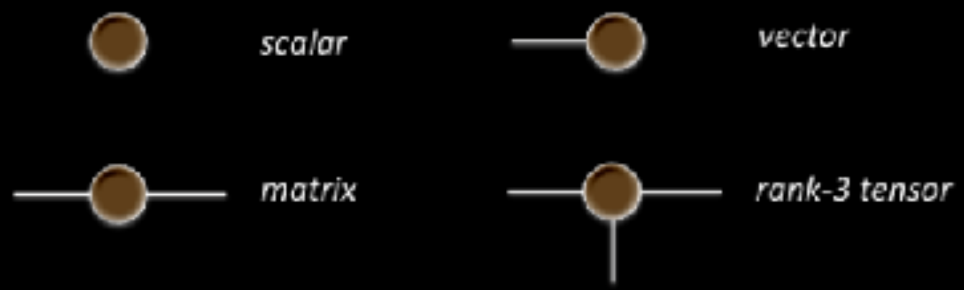

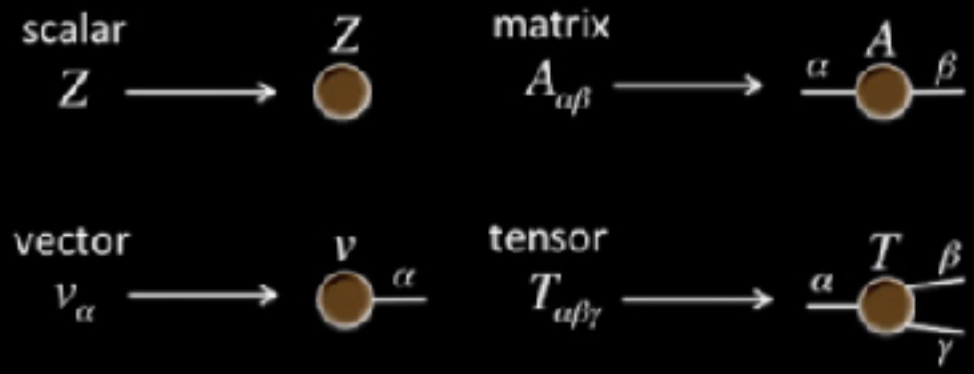

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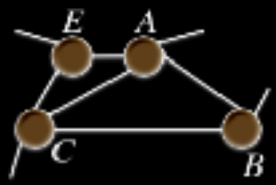
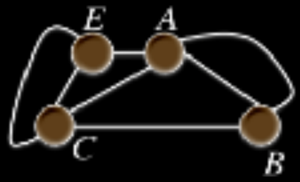
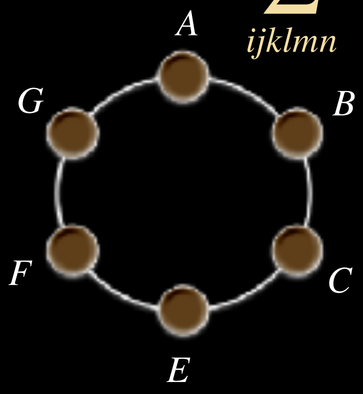


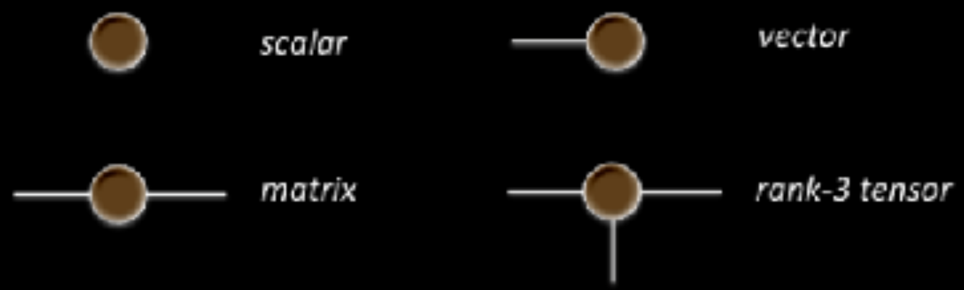


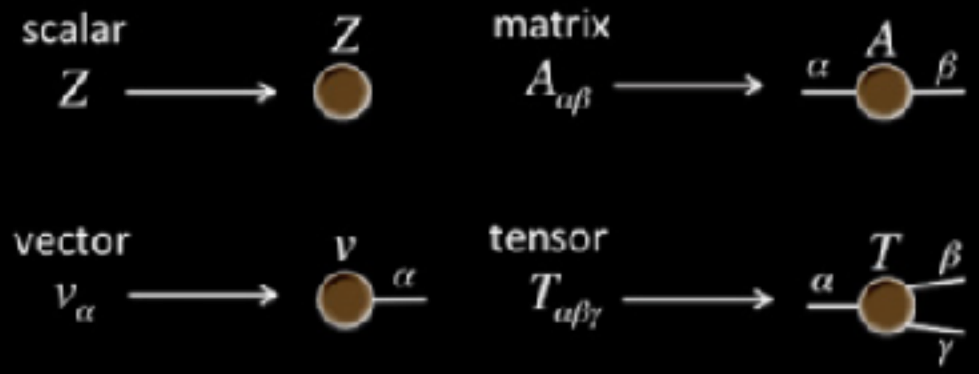
$$\sum_{ijklmnr} A_{ijkl}B_{ijm}C_{kmnr}E_{lknr} = D$$

$$\sum_{ijklmn} A_{ij}B_{jk}C_{kl}E_{lm}F_{mn}G_{ni} = \mathrm{Tr}\,(ABCEFG) = D$$



Tensor Network is a Tensor Product State





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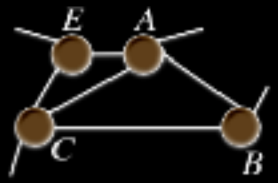

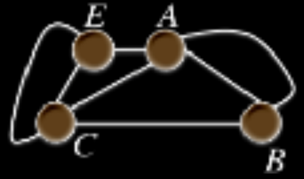

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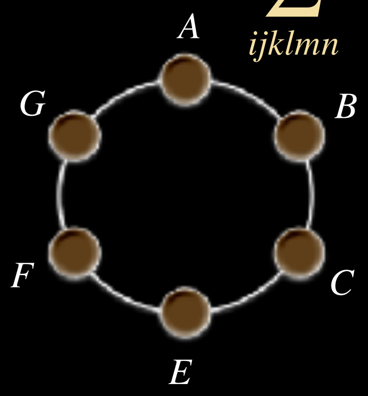

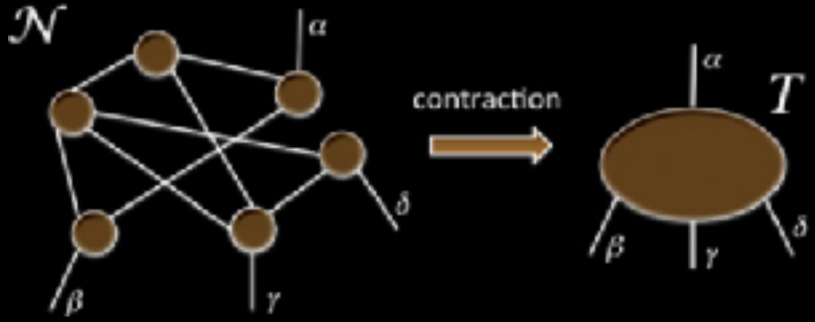

For more details, read the outstanding review by Román Orús

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ANNALS of PHYSICS

A practical introduction to tensor networks: Matrix product states and projected entangled pair states

CrossMark

Román Orús *

Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

Thank you

Matrix *diagonalization*

M *a square matrix* $(n \times n)$

$$M = UDU^{-1}$$

$$M = UDU^{+}$$ *(if Hermitian)*

$$U^{+}U = \mathbb{I}$$

Singular value decomposition

(Schmidt decomposition)

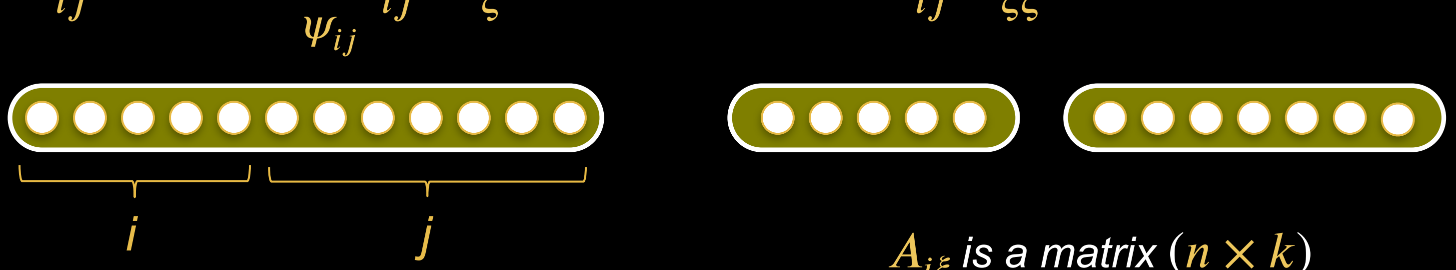
M *is a rectangular matrix* $(n \times m)$

$$M = UDV^{+}$$

$$U^{+}U = V^{+}V = \mathbb{I}$$

Decomposing a vector $|\psi\rangle$ into the product of two matrices A and B

$$|\psi\rangle = \sum_{ij}\psi_{ij}|ij\rangle = \sum_{ij}\sum_{\xi} A_{i\xi}B_{\xi j}|ij\rangle \overset{SVD}{=} \sum_{ij}\sum_{\xi\xi'} U_{i\xi}D_{\xi\xi'}V^{+}_{\xi' j}|ij\rangle$$



ψ_{ij} is a matrix $(n \times m)$

$i = 0,1,2,\ldots,2^n,\;\; j = 0,1,2,\ldots,2^m$

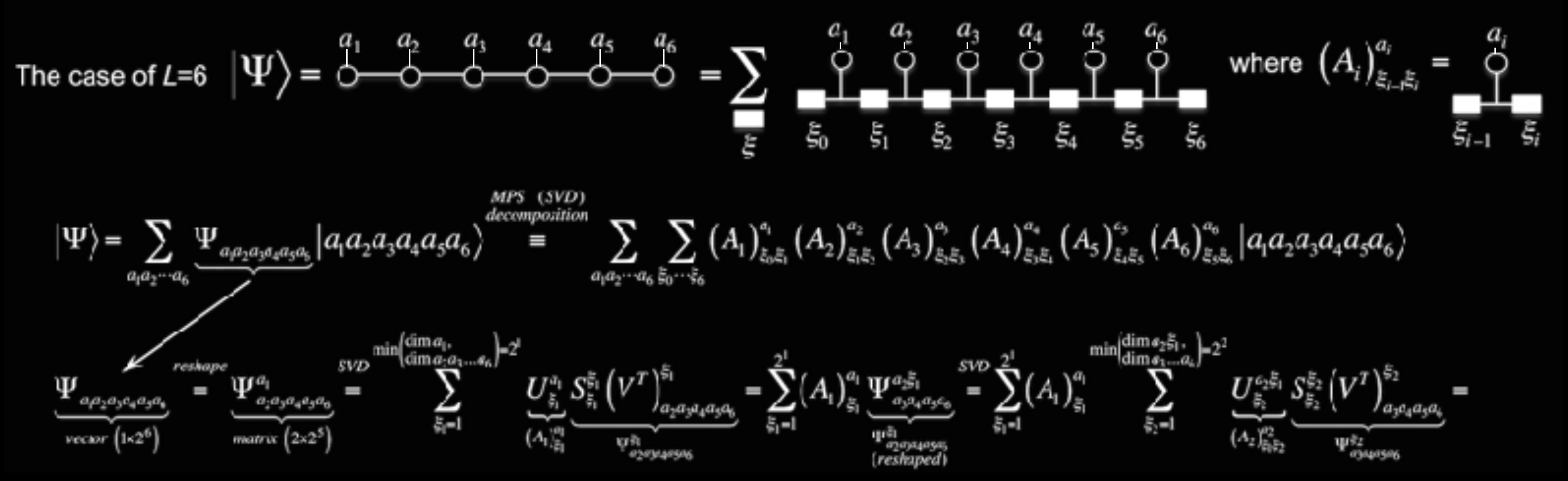
$A_{i\xi}$ is a matrix $(n \times k)$

$B_{\xi j}$ is a matrix $(k \times m)$

$k = \min(n,m)$

$$A_{i\xi} = U_{i\xi}\sqrt{D_{\xi\xi}}$$

$$B_{\xi j} = \sqrt{D_{\xi\xi}}V^{+}_{\xi' j}$$



Singular Value Decomposition (Schmidt decomposition)

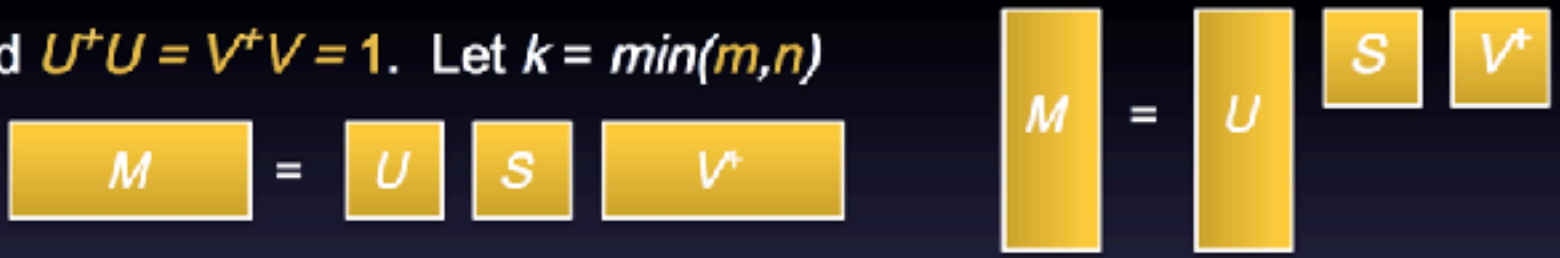
of a $m \times n$ rectangular matrix M is the following decomposition:

$$M = U\,S\,V^{+}$$

U is a unitary $m \times m$ square matrix

S is a diagonal $m \times n$ rectangular matrix (with non-negative real numbers)

and $U^{+}U = V^{+}V = 1$. Let $k = min(m,n)$



The decomposition of a eigenstate Ψ_0 (Schmidt decomposition) onto the product of two matrices A_s and A_e:

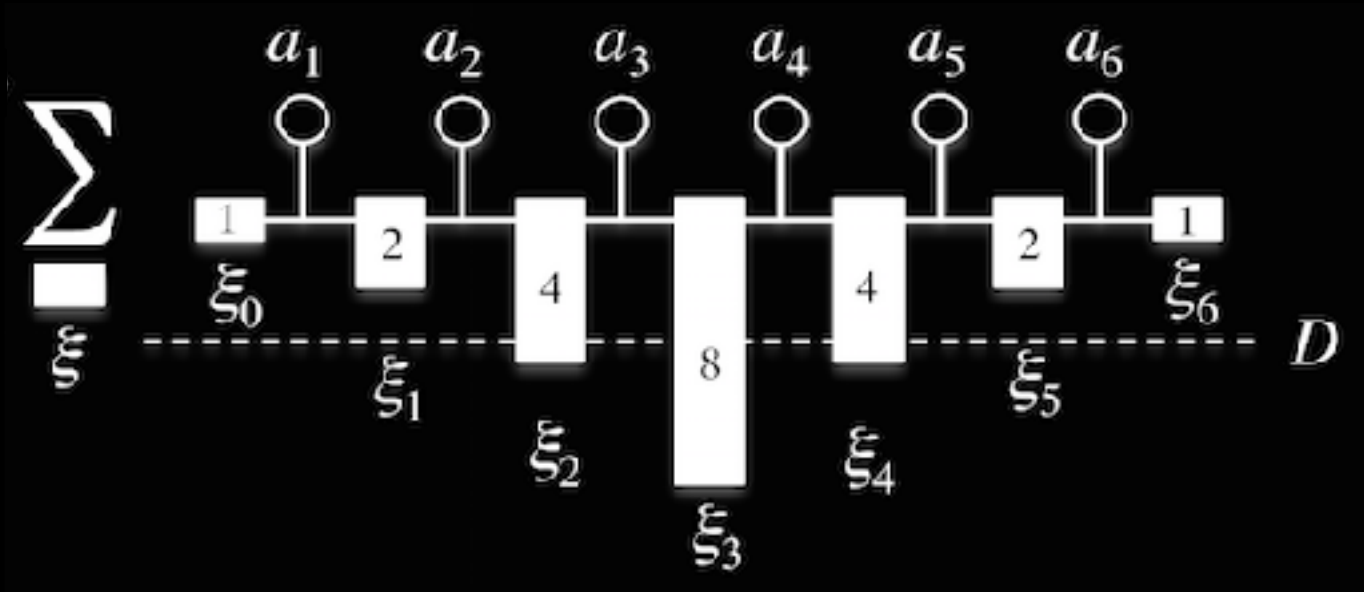
$$|\Psi_0\rangle = \Sigma_{ij}\, \Psi_{ij}\, |i\rangle_s\, |j\rangle_e$$

Analytically:

$$\Psi_0(a_1,a_2,\ldots,a_{L/2},a_{L/2+1},\ldots,a_L) = \Psi^{a_1,a_2,\ldots,a_{L/2}}_{a_{L/2+1},\ldots,a_L} \underset{SVD}{=} \sum_{m}^{D} \underbrace{U^{a_1,a_2,\ldots,a_{L/2}}_{m}}_{A_s} \underbrace{D^{m}_{m} V^{+\,m}_{a_{L/2+1},\ldots,a_L}}_{A_e}$$

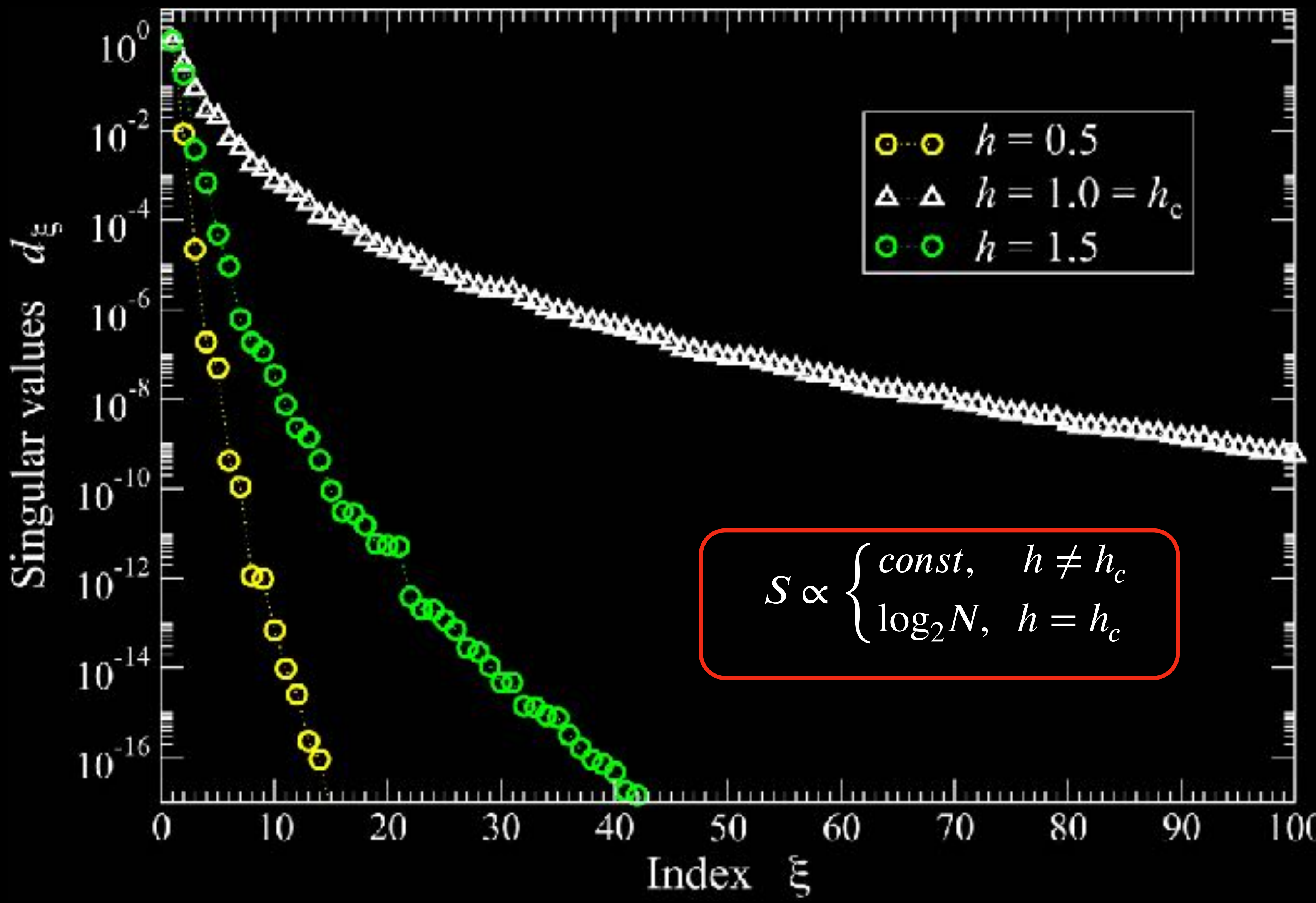
$$|\Psi\rangle = \sum_{a_1 a_2 \cdots a_6} \underbrace{\Psi_{a_1 a_2 a_3 a_4 a_5 a_6}} |a_1 a_2 a_3 a_4 a_5 a_6\rangle \overset{\substack{MPS\ \ (SVD) \\ decomposition}}{\equiv} \sum_{a_1 a_2 \cdots a_6} \sum_{\xi_0 \cdots \xi_6} (A_1)^{a_1}_{\xi_0 \xi_1} (A_2)^{a_2}_{\xi_1 \xi_2} (A_3)^{a_3}_{\xi_2 \xi_3} (A_4)^{a_4}_{\xi_3 \xi_4} (A_5)^{a_5}_{\xi_4 \xi_5} (A_6)^{a_6}_{\xi_5 \xi_6} |a_1 a_2 a_3 a_4 a_5 a_6\rangle$$

=

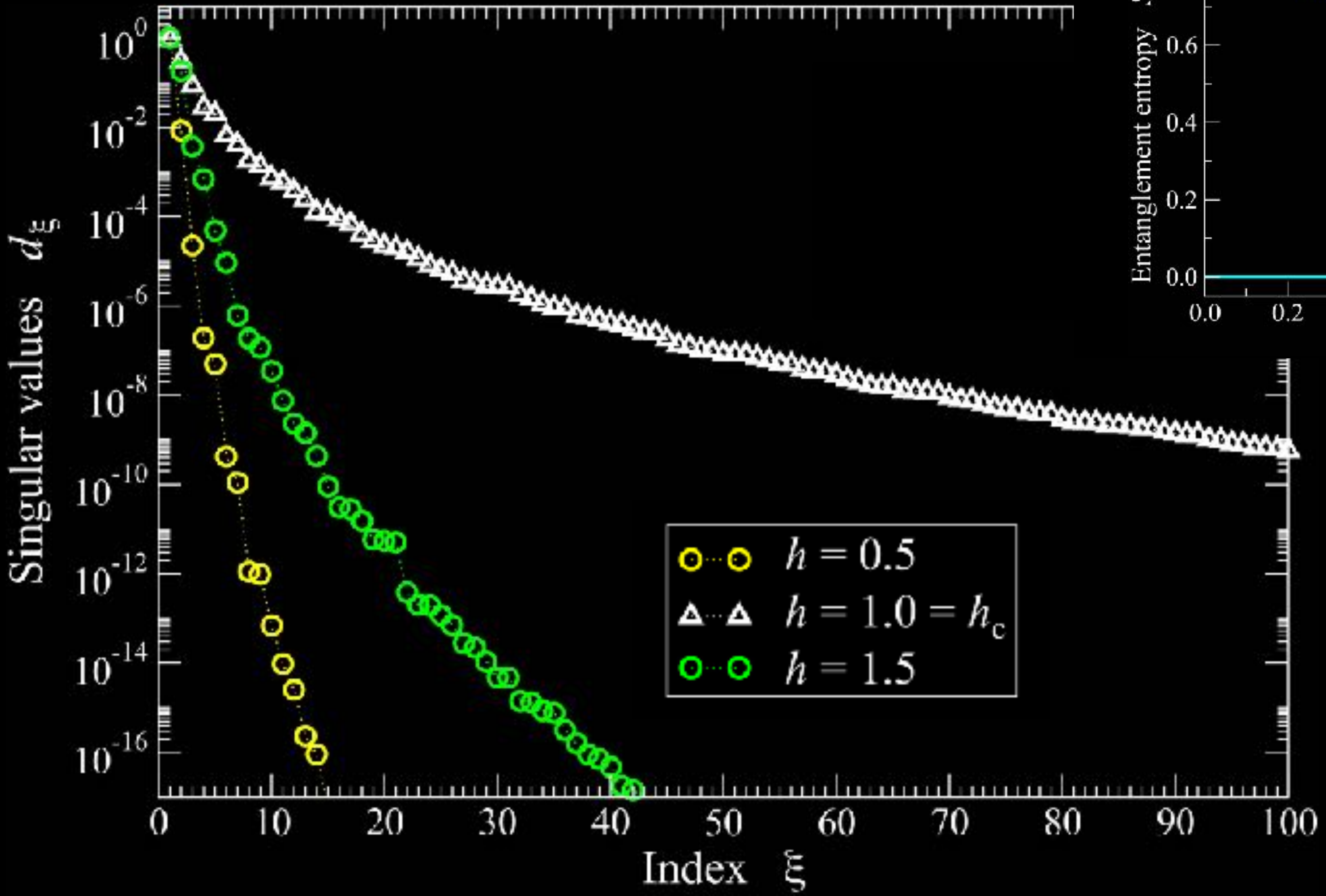


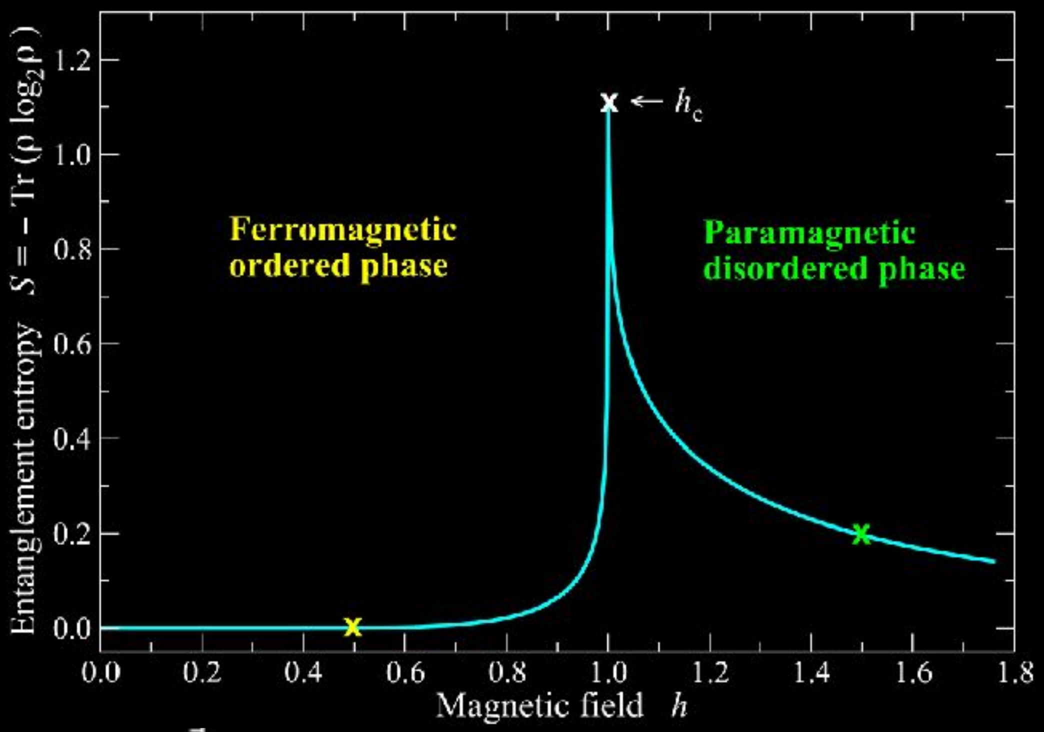
More details on singular value decomposition in 1D chain of 6 spins

Decay of the singular values (Schmidt coefficients) d_ξ



$$S \propto \begin{cases} const, & h \neq h_c \\ \log_2 N, & h = h_c \end{cases}$$


Singular values d_ξ
Index ξ
$h = 0.5$
$h = 1.0 = h_c$
$h = 1.5$


Entanglement entropy $S = -\mathrm{Tr}\,(\rho \log_2 \rho)$
Magnetic field h
$\leftarrow h_c$
Ferromagnetic ordered phase
Paramagnetic disordered phase

The case of L=6 $|\Psi\rangle =$  $= \sum_{\xi}$  where $(A_i)^{a_i}_{\xi_{i-1}\xi_i} =$ 

$$|\Psi\rangle = \sum_{a_1a_2\cdots a_6} \underbrace{\Psi_{a_1a_2a_3a_4a_5a_6}}\,|a_1a_2a_3a_4a_5a_6\rangle \overset{\substack{MPS\ (SVD)\\ decomposition}}{=} \sum_{a_1a_2\cdots a_6}\sum_{\xi_0\cdots\xi_6}(A_1)^{a_1}_{\xi_0\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5\xi_6}|a_1a_2a_3a_4a_5a_6\rangle$$

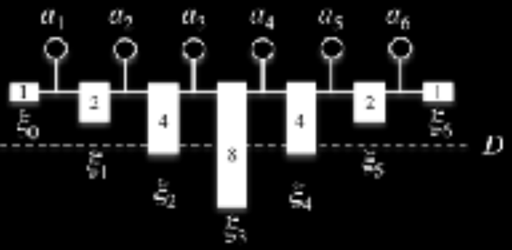
$$\underbrace{\Psi_{a_1a_2a_3a_4a_5a_6}}_{vector\ (1\times 2^6)} \overset{reshape}{=} \underbrace{\Psi^{a_1}_{a_2a_3a_4a_5a_6}}_{matrix\ (2\times 2^5)} \overset{SVD}{=} \sum_{\xi_1=1}^{\min\left(\substack{\dim a_1,\\ \dim a_2a_3\ldots a_6}\right)=2^1} \underbrace{U^{a_1}_{\xi_1}}_{(A_1)^{a_1}_{\xi_1}}\underbrace{S^{\xi_1}_{\xi_1}\left(V^T\right)^{\xi_1}_{a_2a_3a_4a_5a_6}}_{\Psi^{\xi_1}_{a_2a_3a_4a_5a_6}} = \sum_{\xi_1=1}^{2^1}(A_1)^{a_1}_{\xi_1}\underbrace{\Psi^{a_2\xi_1}_{a_3a_4a_5a_6}}_{\substack{\Psi^{\xi_1}_{a_2a_3a_4a_5a_6}\\ (reshaped)}} \overset{SVD}{=} \sum_{\xi_1=1}^{2^1}(A_1)^{a_1}_{\xi_1}\sum_{\xi_2=1}^{\min\left(\substack{\dim a_2\xi_1,\\ \dim a_3\ldots a_6}\right)=2^2}\underbrace{U^{a_2\xi_1}_{\xi_2}}_{(A_2)^{a_2}_{\xi_1\xi_2}}\underbrace{S^{\xi_2}_{\xi_2}\left(V^T\right)^{\xi_2}_{a_3a_4a_5a_6}}_{\Psi^{\xi_2}_{a_3a_4a_5a_6}} =$$

$$= \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}\underbrace{\Psi^{a_3\xi_2}_{a_4a_5a_6}}_{\substack{\Psi^{\xi_2}_{a_3a_4a_5a_6}\\ (reshaped)}} \overset{SVD}{=} \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}\sum_{\xi_3=1}^{\min\left(\substack{\dim a_3\xi_2,\\ \dim a_4a_5a_6}\right)=2^3}\underbrace{U^{a_3\xi_2}_{\xi_3}}_{(A_3)^{a_3}_{\xi_2\xi_3}}\underbrace{S^{\xi_3}_{\xi_3}\left(V^T\right)^{\xi_3}_{a_4a_5a_6}}_{\Psi^{\xi_3}_{a_4a_5a_6}} = \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}\underbrace{\Psi^{a_4\xi_3}_{a_5a_6}}_{\substack{\Psi^{\xi_3}_{a_4a_5a_6}\\ (reshaped)}} \overset{SVD}{=}$$

$$\overset{SVD}{=} \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}\sum_{\xi_4=1}^{\min\left(\substack{\dim a_4\xi_3,\\ \dim a_5a_6}\right)=2^2}\underbrace{U^{a_4\xi_3}_{\xi_4}}_{(A_4)^{a_4}_{\xi_3\xi_4}}\underbrace{S^{\xi_4}_{\xi_4}\left(V^T\right)^{\xi_4}_{a_5a_6}}_{\Psi^{\xi_4}_{a_5a_6}} = \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}\underbrace{\Psi^{a_5\xi_4}_{a_6}}_{\substack{\Psi^{\xi_4}_{a_5a_6}\\ (reshaped)}} \overset{SVD}{=}$$

$$\overset{SVD}{=} \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}\sum_{\xi_5=1}^{\min\left(\substack{\dim a_5\xi_4,\\ \dim a_6}\right)=2^1}\underbrace{U^{a_5\xi_4}_{\xi_5}}_{(A_5)^{a_5}_{\xi_4\xi_5}}\underbrace{S^{\xi_5}_{\xi_5}\left(V^T\right)^{\xi_5}_{a_6}}_{\Psi^{\xi_5}_{a_6}=(A_6)^{a_6}_{\xi_5}} = \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}\sum_{\xi_5=1}^{2^1}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5}$$

$$\overset{in\ general}{=} \sum_{\xi_0=1}^{2^0}\sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}\sum_{\xi_5=1}^{2^1}\sum_{\xi_6=1}^{2^0}(A_1)^{a_1}_{\xi_0\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5\xi_6} \overset{graphically}{=} \sum_{\xi}$$



$$\overset{(D<2^{L/2})}{\approx} \sum_{\xi_0=1}^{D}\sum_{\xi_1=1}^{D}\sum_{\xi_2=1}^{D}\sum_{\xi_3=1}^{D}\sum_{\xi_4=1}^{D}\sum_{\xi_5=1}^{D}\sum_{\xi_6=1}^{D}(A_1)^{a_1}_{\xi_0\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5\xi_6}$$

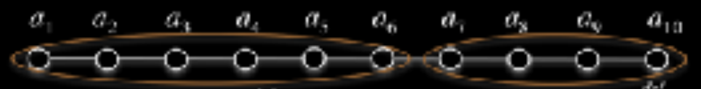
For any finite L

$$|\Psi\rangle = \sum_{a_1 a_2 \cdots a_L} \Psi_{a_1 a_2 \cdots a_L} |a_1 a_2 \cdots a_L\rangle \overset{\substack{MPS\ (SVD)\\ decomposition}}{=} \sum_{a_1 a_2 \cdots a_L} \sum_{\xi_0 \cdots \xi_L} \prod_{i=1}^{L} (A_i)^{a_i}_{\xi_{i-1}\xi_i} |a_1 a_2 \cdots a_L\rangle$$

$$= \sum_{a_1 a_2 \cdots a_L} \sum_{\xi_0=1}^{2^0} \sum_{\xi_1=1}^{2^1} \cdots \sum_{\xi_{L/2-1}=1}^{2^{L/2-1}} \sum_{\xi_{L/2}=1}^{2^{L/2}} \sum_{\xi_{L/2+1}=1}^{2^{L/2+1}} \cdots \sum_{\xi_L=1}^{2^0} \prod_{i=1}^{L} (A_i)^{a_i}_{\xi_{i-1}\xi_i} |a_1 a_2 \cdots a_L\rangle \overset{(D \ll 2^{L/2})}{\approx} \sum_{a_1 a_2 \cdots a_L} \sum_{\xi_0 \cdots \xi_L}^{D} \prod_{i=1}^{L} (A_i)^{a_i}_{\xi_{i-1}\xi_i} |a_1 a_2 \cdots a_L\rangle$$

Note that $\dim\left\{(A_i)^{a_i}_{\xi_{i-1}\xi_i}\right\} = qD^2$, where, e.g., $q = \begin{cases} 2 & \textit{Heisenberg}, \\ 4 & \textit{Hubbard}. \end{cases}$

Consider spinless electrons on a linear chain with a finite length L divided into two parts with sizes k and $L-k$, where ($1 \le k \le L-1$). We show that von Neumann entanglement entropies S_{sys} and S_{env} for both of the chains are <u>identical</u> for a fixed k.



$$|a_1 a_2 \cdots a_{k=6}\rangle_{system} \overset{def}{=} |i\rangle_{sys} \qquad |a_{k+1} \cdots a_L\rangle_{environment} \overset{def}{=} |j\rangle_{env}$$

$$S_{\substack{sys\\env}} = -Tr\left(\rho_{\substack{sys\\env}} \log_2 \rho_{\substack{sys\\env}}\right)$$

$$\rho_{sys} = Tr_{env}|\Psi\rangle\langle\Psi| = \sum_j \Psi_{ij}\Psi^*_{ji}$$

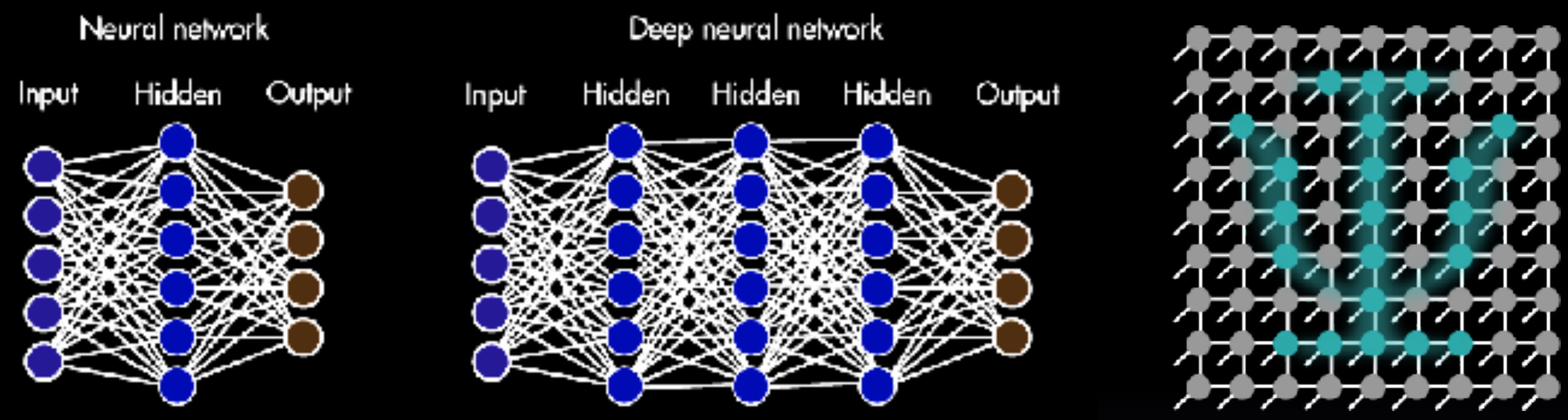
$$\rho_{env} = Tr_{sys}|\Psi\rangle\langle\Psi| = \sum_i \Psi^*_{ji}\Psi_{ij}$$

$$|\Psi\rangle = \sum_{i=1}^{2^k}\sum_{j=1}^{2^{L-k}} \Psi^i_j |i\rangle_{sys}|j\rangle_{env} \overset{SVD}{=} \sum_{i=1}^{2^k}\sum_{j=1}^{2^{L-k}} \sum_{\xi=1}^{m=\min(2^k,2^{L-k})} U^i_\xi \underbrace{S^\xi_\xi}_{\substack{m_\xi\\ diag.\\ matrix}} \left(V^T\right)^\xi_j |i\rangle_{sys}|j\rangle_{env} = \sum_{\xi=1}^{m} s_\xi \underbrace{\sum_{i=1}^{2^k} U^i_\xi |i\rangle_s}_{=|\xi\rangle_{sys}} \underbrace{\sum_{j=1}^{2^{L-k}} \left(V^T\right)^\xi_j |j\rangle_e}_{=|\xi\rangle_{env}} = \sum_{\xi=1}^{m} s_\xi |\xi\rangle_{sys}|\xi\rangle_{env}$$

$$\rho_{sys} = Tr_{env}|\Psi\rangle\langle\Psi| = \sum_{j=1}^{2^{L-k}}\sum_{\xi=1}^{m} s_\xi |\xi\rangle_{sys}|\xi\rangle_{env} \sum_{\eta=1}^{m}\left[s_\eta|\eta\rangle_{sys}|\eta\rangle_{env}\right]^+ = \sum_{\xi=1}^{m}\sum_{\eta=1}^{m} \underbrace{s_\xi s^*_\eta}_{s^*_\eta = s_\eta} |\xi\rangle_{sys} \underbrace{\sum_{j=1}^{2^{L-k}} |\xi\rangle_{env}\langle\eta|_{env}}_{=\delta_{\xi,\eta}} \langle\eta|_{sys} = \sum_{\xi=1}^{m} s^2_\xi |\xi\rangle_{sys}\langle\xi|_{sys}$$

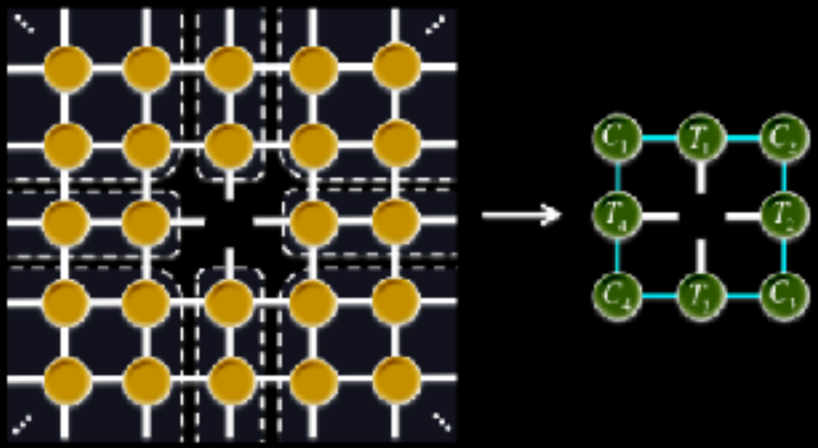
$$\rho_{env} = Tr_{sys}|\Psi\rangle\langle\Psi| = \sum_{i=1}^{2^k}\sum_{\xi=1}^{m}\left[s_\xi|\xi\rangle_{sys}|\xi\rangle_{env}\right]^+ \sum_{\eta=1}^{m} s_\eta|\eta\rangle_{sys}|\eta\rangle_{env} = \sum_{\xi=1}^{m}\sum_{\eta=1}^{m} \underbrace{s^+_\xi s_\eta}_{s^+_\xi = s_\xi} |\xi\rangle_{env} \underbrace{\sum_{i=1}^{2^k} |\xi\rangle_{sys}\langle\eta|_{sys}}_{=\delta_{\xi,\eta}} \langle\eta|_{env} = \sum_{\xi=1}^{m} s^2_\xi |\xi\rangle_{env}\langle\xi|_{env}$$

For any fixed k, even if $k \neq L/2$, we get $\left\{\begin{array}{l} S_{sys} = -Tr_{sys}\left(\rho_{sys}\log_2\rho_{sys}\right) = \sum_{\xi=1}^{m} s^2_\xi \log_2\left(s^2_\xi\right) \\ S_{env} = -Tr_{env}\left(\rho_{env}\log_2\rho_{env}\right) = \sum_{\xi=1}^{m} s^2_\xi \log_2\left(s^2_\xi\right) \end{array}\right\} \rightarrow \boxed{S_{sys} = S_{env}}$

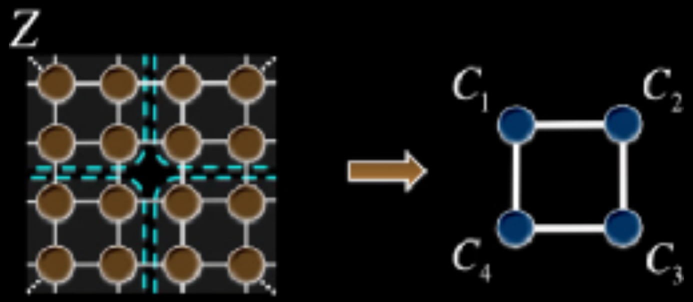

Neural network
Input
Hidden
Output
Deep neural network
Input
Hidden
Hidden
Hidden
Output

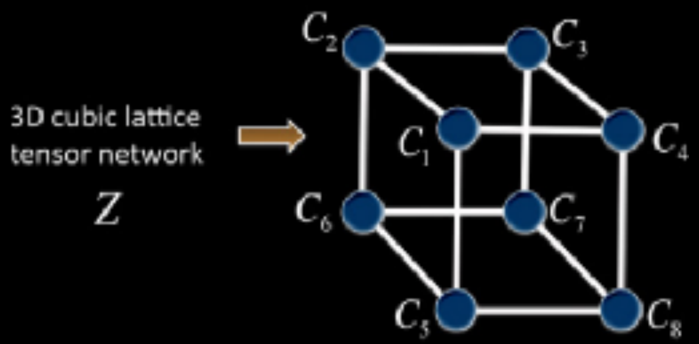
***Tensor Network* is a Tensor Product State**

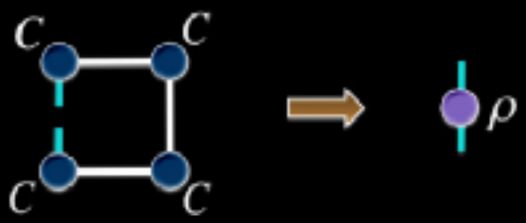
(and it's like playing a Tetris game...)



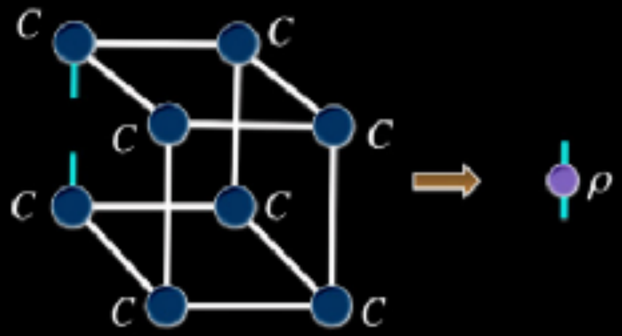
2D Tensor Network
for
Corner Transfer Matrix
Renormalization Group







reduced density matrix



reduced density matrix

Reduced density matrix

Let us start by finding spectrum of energies E_n and the corresponding eigenstates $|\psi_n\rangle$ of a given Hamiltonian (that is how the QM works)

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

- Reduced density matrix in a pure state $\rho' = Trenv\left(|\psi_0\rangle\langle\psi_0|\right)$
- Reduced density matrix in a mixed state

$$\rho'' = Trenv\left(\sum_j c_j|\psi_j\rangle\langle\psi_j|\right)$$

- What is the reduced density matrix typically good for?
  - ✓ To obtain expectation (mean) values of operators $\langle As\rangle = Trs\left(As\rho'\right)$
  - ✓ Quantum entanglement von Neumann entropy

Information inside the reduced density matrix

The reduced density matrix completely describes a subsystem (in contact with environment).

Properties of the entanglement entropy:

$$S = -Tr_s\left(\rho_s' \log_2 \rho_s'\right) \geq 0$$

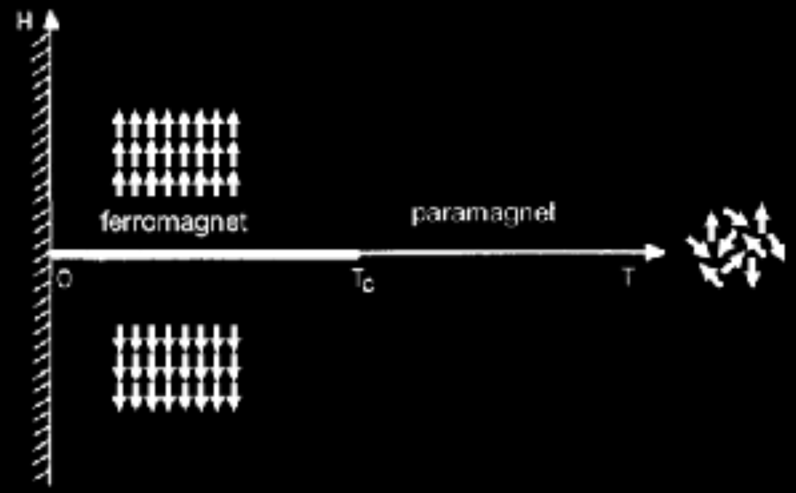
If the reduced density matrix is diagonalized $U^{+}\rho_s' U = \Omega,$

the eigenvalues sorted in descending order are: $\omega 1 \geq \omega 2 \geq \omega 3 \geq \ldots \geq \omega N$

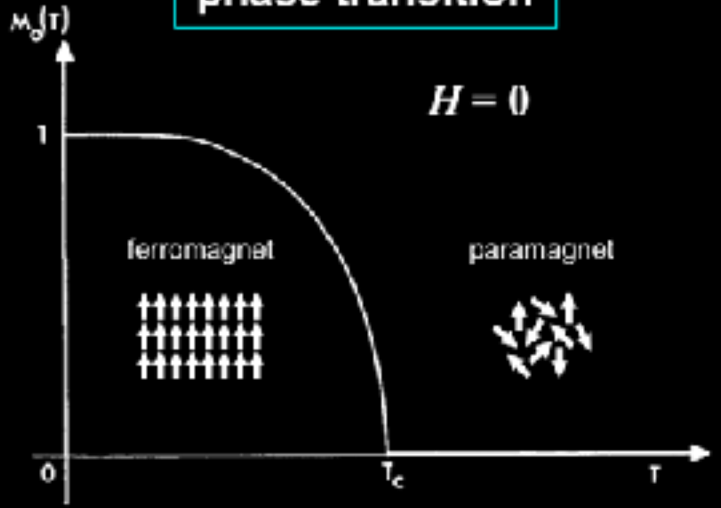
$$U^{+}\rho_s' U = \Omega = \begin{pmatrix} \omega_1 & 0 & 0 & \\ 0 & \omega_2 & 0 & \cdots \\ 0 & 0 & \omega_3 & \\ & \vdots & & \ddots & \\ & & & & \omega_N \end{pmatrix}$$

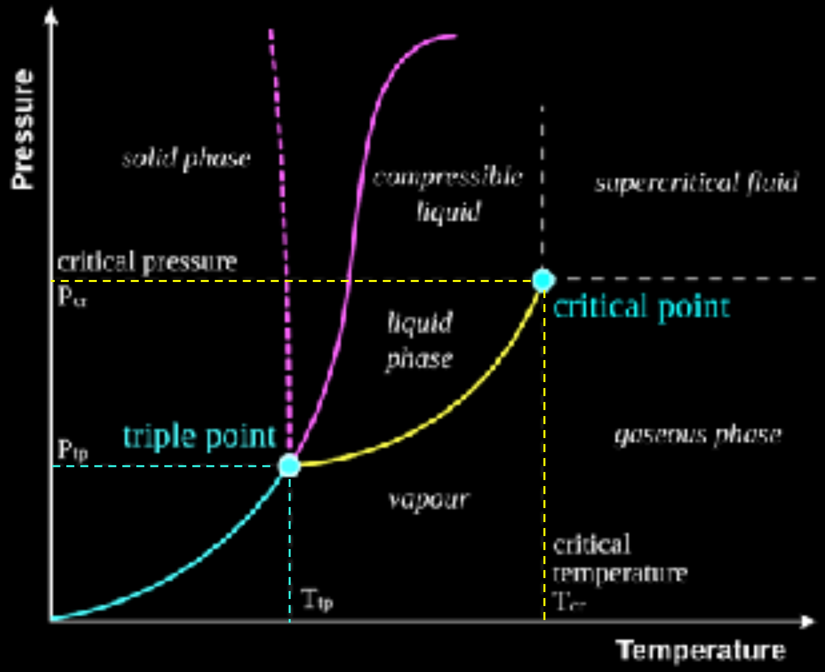
- ✓ No entanglement: $\omega 1 = 1, \ \omega j = 0, \ \forall j > 1$
- ✓ Weak entanglement: $\omega j \propto \exp(-\beta j)$
- ✓ Strong entanglement: $\omega j \propto j^{-\alpha}$

Phase transitions



The 2nd order phase transition





The 1st order phase transition